

# *FT-IETS and Bosonic Function in High-T<sub>c</sub> Superconductors*

## *Motivation:*

- Spectroscopy technique
- Properties of electron-boson interaction at nanoscale in real-space: local/delocalized ?
- For anisotropic electron-boson interaction, measure directly momentum transfer  $\vec{q}$  and energy  $\Omega_0$
- Ideally find the anisotropic electron-boson spectral density  $\alpha^2(\vec{q}, \Omega)F(\vec{q}, \Omega)$

### *Collaborators:*

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Q. Si(Rice), Jinho Lee, Kyle  
McElroy, JC Davis(Cornell)

# MOLECULAR VIBRATION SPECTRA BY ELECTRON TUNNELING

R. C. Jaklevic and J. Lambe

Scientific Laboratory, Ford Motor Company, Dearborn, Michigan

(Received 18 October 1966)

The conductance of metal-metal oxide-metal tunneling junctions has been observed to increase at certain characteristic bias voltages. These voltages are identified with vibrational frequencies of molecules contained in the barrier.

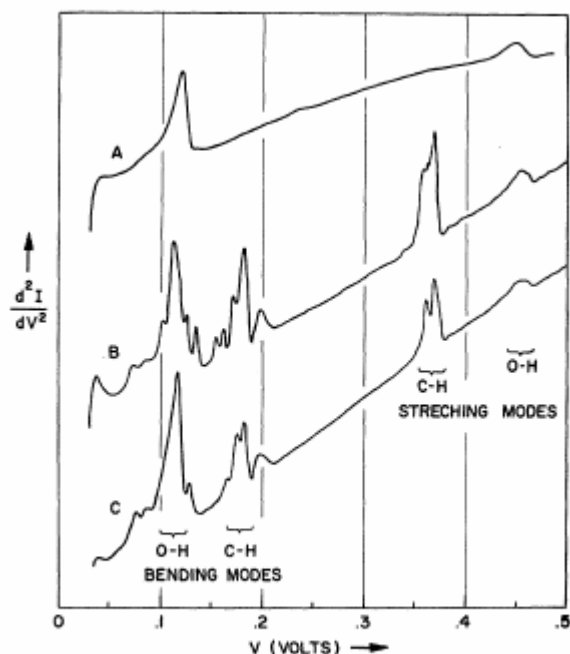
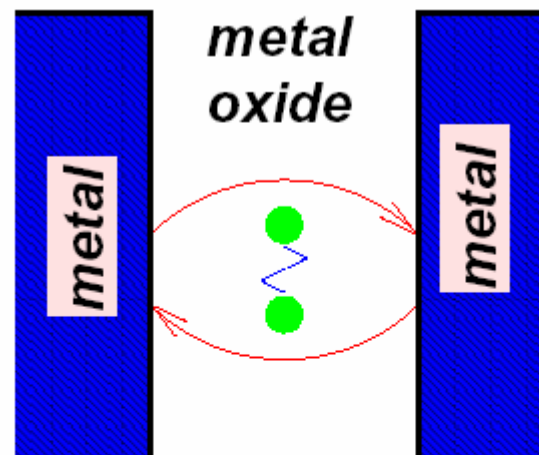


FIG. 1. Recorder traces of  $d^2I/dV^2$  versus applied voltage for three Al-Al oxide-Pb junctions taken at

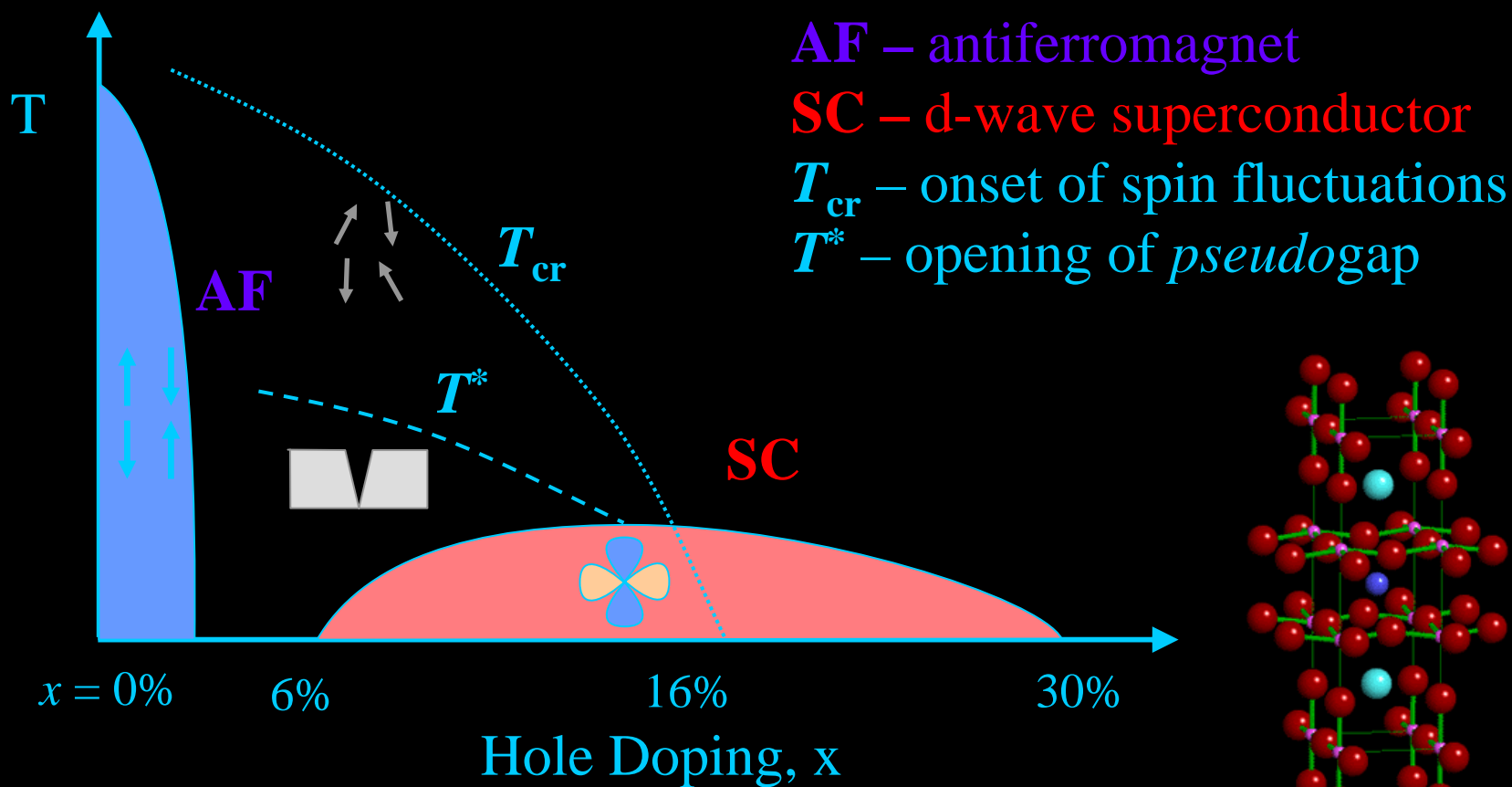


$$H_t = c_L^\dagger c_R T(x) + h.c.$$

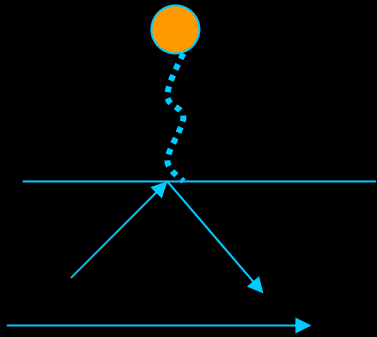
$$T(x) = t_0(1 + \alpha x)$$

$$x = \text{Vibrational mode}$$

# Experimental Phase Diagram



# Inelastic tunneling spectroscopy in a metal



$$H = H + \frac{kx^2}{2} + gc_{\sigma}^*(r=0)c_{\sigma}(r=0)x$$

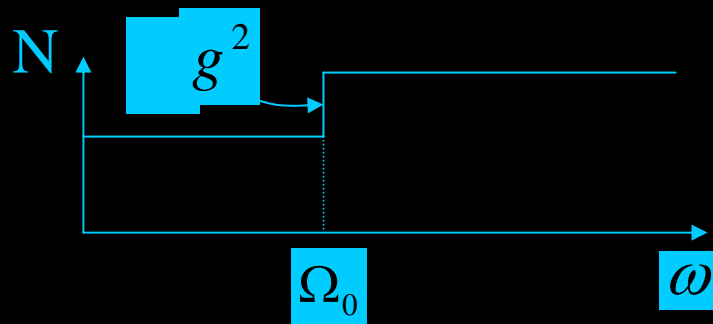
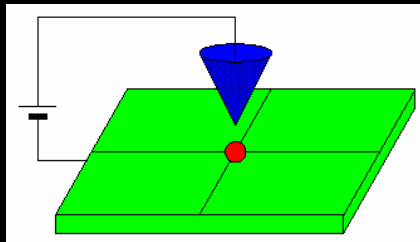
Self-energy  $\Sigma(\omega) = g^2 G(r=0, \omega) * D(\omega)$

$$\delta N(r, \omega) = \frac{1}{\pi} \text{Im}[G^0(r, \omega) \Sigma(\omega) G^0(r, \omega)]$$



$\Sigma(\omega)$

$$\delta N(r, \omega) \sim g^2 N_0 (\omega - \Omega_0) \Theta(\omega - \Omega_0)$$



For a metal

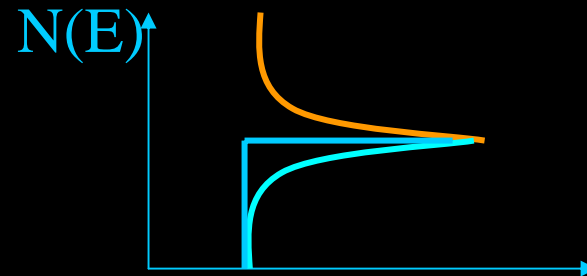
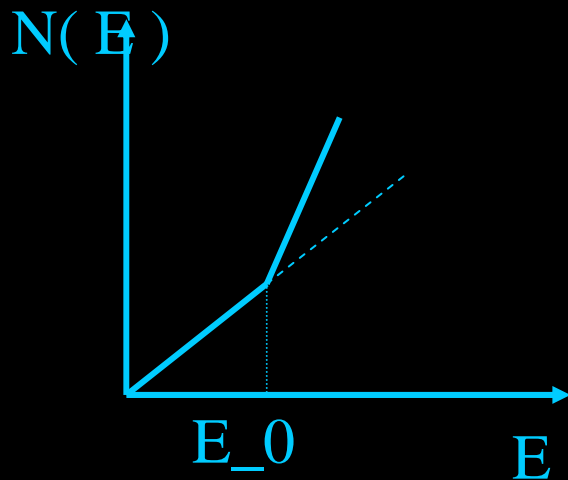
## Second order analysis

For a d-wave or a pseudo-gapped state feature will be much smaller

$$\delta N(r, \omega) \sim g^2 (\omega - \Omega_0)^\gamma \Theta(\omega - \Omega_0)$$

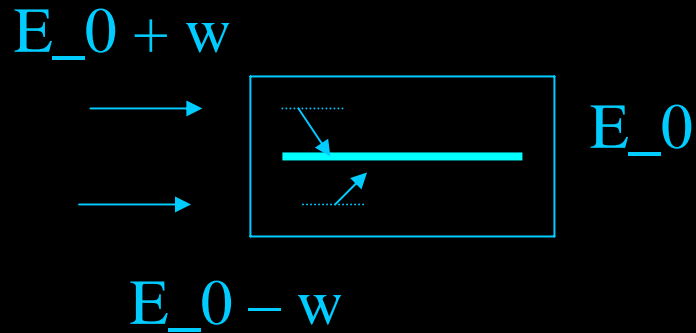
where  $\gamma$  is the DOS power

$$\frac{d^2 I}{dV^2} \sim g^2 (\omega - \Omega_0)^{\gamma-1} \Theta(\omega - \Omega_0)$$

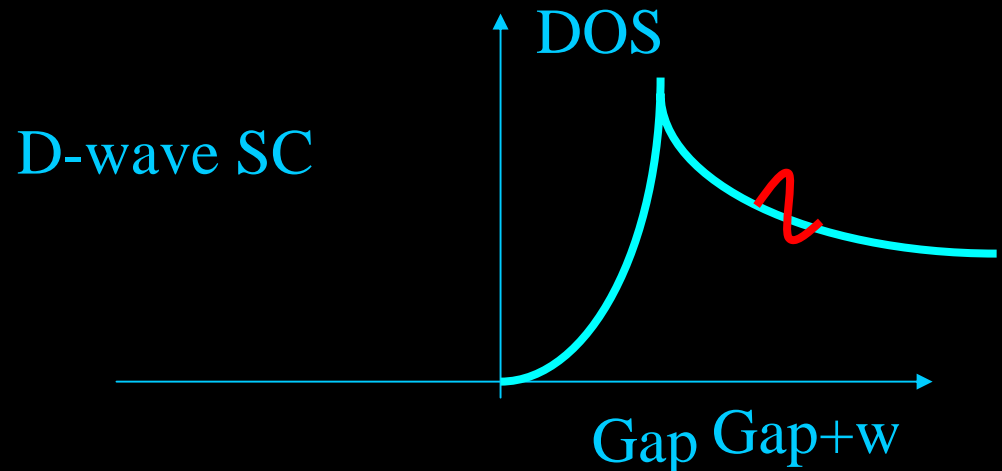
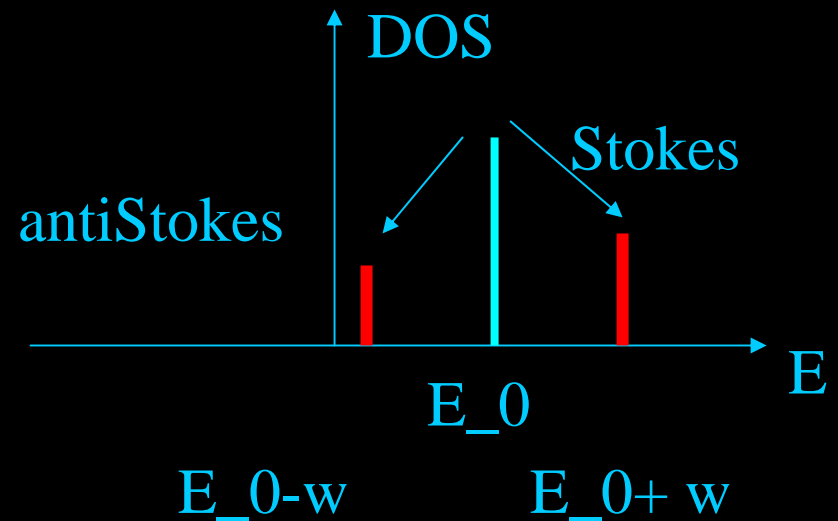


Similar to x-ray absorption singularity

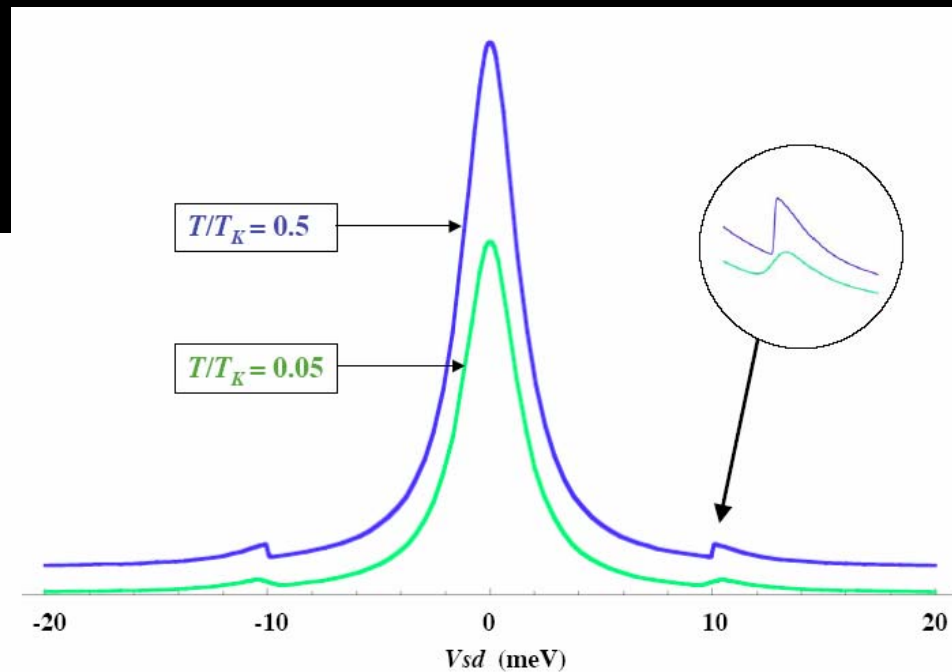
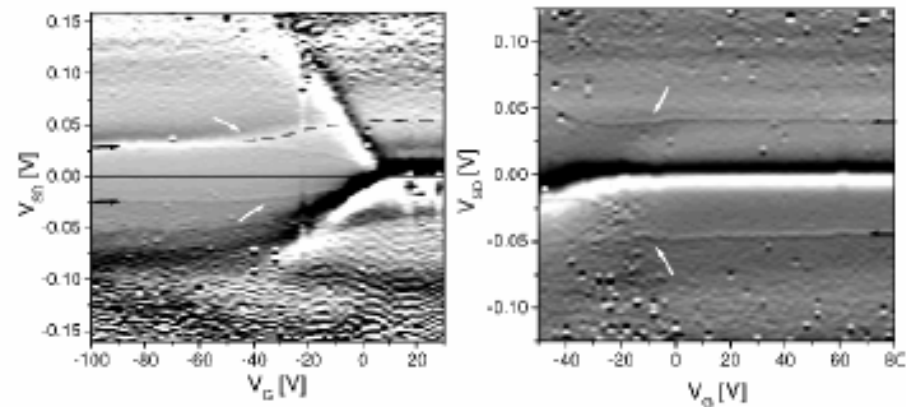
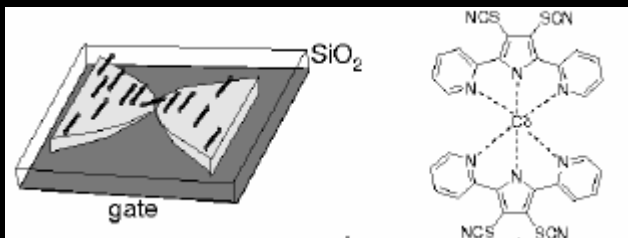
# *Inelastic scattering induced satellites: Holstein effects*



At finite  $T$  there is a probability that local mode is excited



# *Inelastic satellites to Kondo peak in molecular devices*



D. Natelson et al, cond-mat 0408052

Abrahams and AVB, preprint

Korea workshop, Feb 2005

# Inelastic Tunneling Spectroscopy in a D-wave Superconductor.

A.V. Balatsky, Ar. Abanov, and Jian-Xin Zhu

PRB, sept 2003

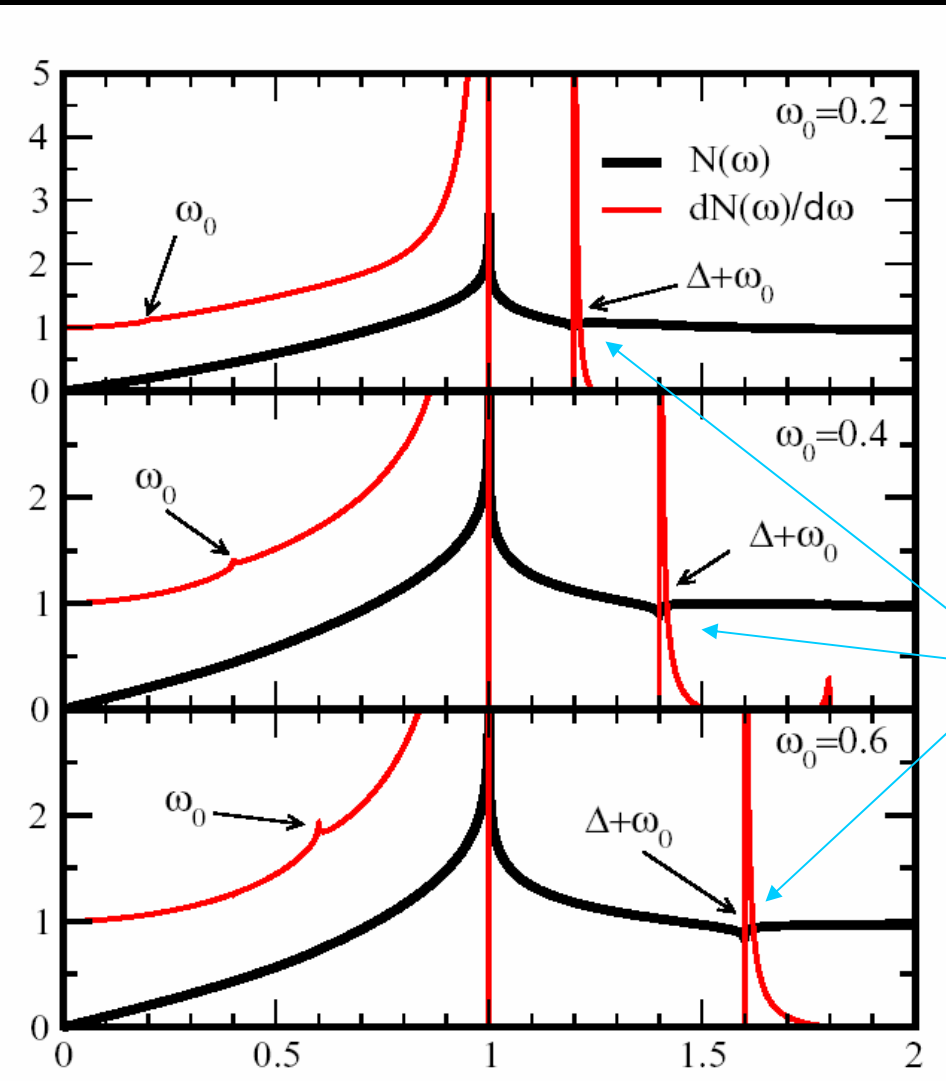
$$H = \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} \epsilon(\mathbf{k}) c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\Delta(\mathbf{k}) c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} + h.c.) \\ + \sum_{\mathbf{k}, \mathbf{k}', \sigma, \sigma'} JS \cdot c_{\mathbf{k}\sigma}^{\dagger} \boldsymbol{\sigma}_{\sigma\sigma'} c_{\mathbf{k}'\sigma'} + g\mu_B \mathbf{S} \cdot \mathbf{B} ,$$

$$\Sigma(\omega_l) = J^2 T \sum_{\mathbf{k}, \Omega_n} G(\mathbf{k}, \omega_l - \Omega_n) \chi^{+-}(\Omega_n)$$

$$\frac{\delta N(\mathbf{r}=0, \omega)}{N_0} = \frac{\pi^2}{2} (JSN_0)^2 \frac{\omega - \omega_0}{\Delta} K(T, \omega, \omega_0) \\ \times \left( \frac{2\omega}{\Delta} \ln \left( \frac{\Delta}{\omega} \right) \right)^2, \quad \omega \ll \Delta, \quad (6)$$

$$\frac{\delta N(\mathbf{r}=0, \omega)}{N_0} = 2\pi^2 (JSN_0)^2 K(T, \omega, \omega_0) \ln^2 \left( \frac{|\omega - \Delta|}{4\Delta} \right) \\ \times \ln \left( \frac{4\Delta}{|\omega + \omega_0 - \Delta|} \right) + (\omega_0 \rightarrow -\omega_0), \quad \omega \simeq |\Delta|, \quad (7)$$

# Selfconsistent solution for a local vibrational mode



Black line - DOS

Red line- DOS derivative

For  $N_0 \sim 1/eV$ ,  $JN_0 = 0.14$

$$\frac{\delta N}{N_0} \sim (JN_0)^2 \frac{\omega - \Omega_0}{\Delta_0}$$

Holstein features

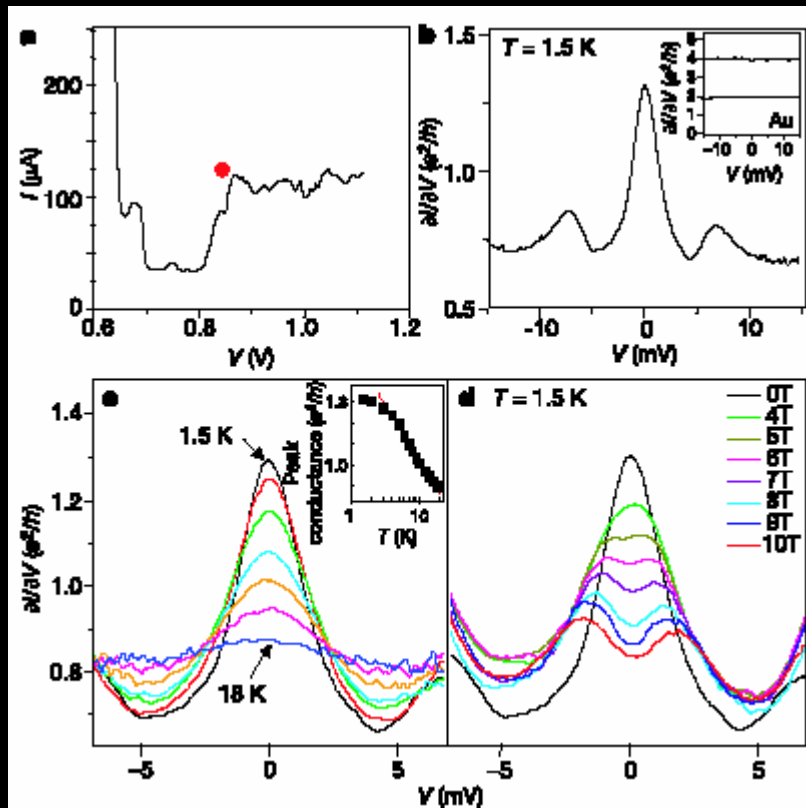
For relative change  
compared to d-wave DOS  
effect is few percent

Inelastic Tunneling Spectroscopy in a D-wave Superconductor.

A.V. Balatsky, Ar. Abanov, and Jian-Xin Zhu

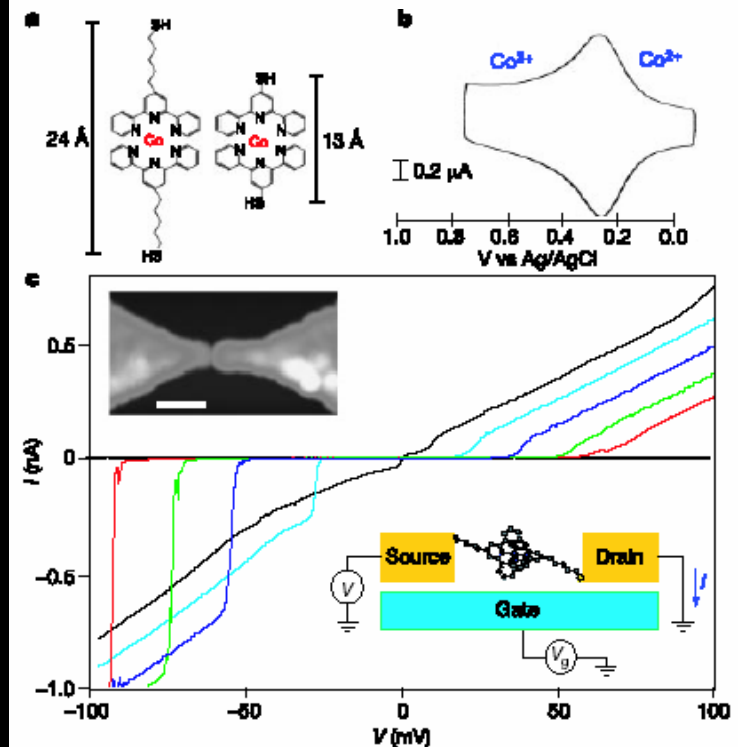
PRB 68 214506 (2003).

# Kondo effect and spin flip spectroscopy in a single atom



## Coulomb blockade and the Kondo effect in single-atom transistors

Jiwoong Park<sup>†,‡</sup>, Abhay N. Pasupathy<sup>†,‡</sup>, Jonas I. Goldsmith<sup>§</sup>,  
 Connie Chang<sup>\*</sup>, Yuval Yaish<sup>\*</sup>, Jason R. Petta<sup>\*</sup>, Marie Rinkoski<sup>\*</sup>,  
 James P. Sethna<sup>\*</sup>, Héctor D. Abruña<sup>§</sup>, Paul L. McEuen<sup>\*</sup> & Daniel C. Ralph<sup>\*</sup>

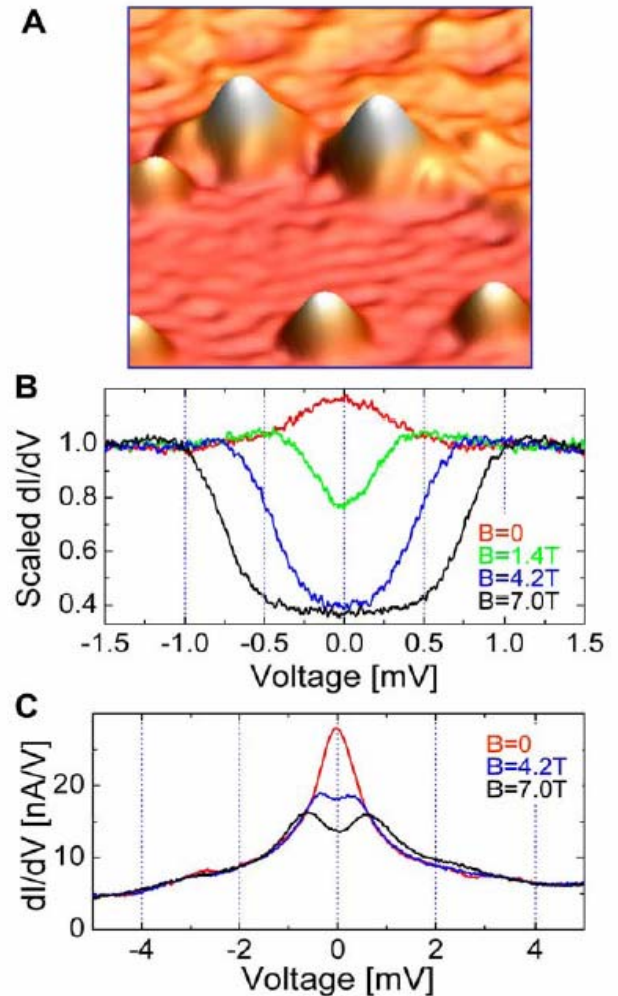
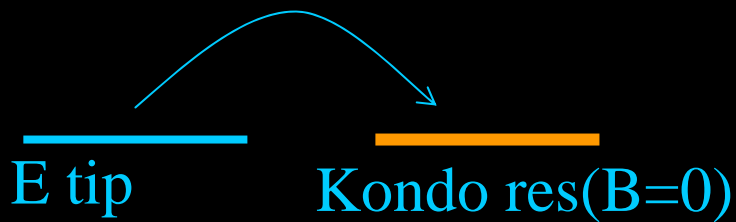


# Single Spin Flip Spectroscopy

Scienceexpress

## Single-Atom Spin-Flip Spectroscopy

A. J. Heinrich,\* J. A. Gupta, C. P. Lutz, D. M. Eigler

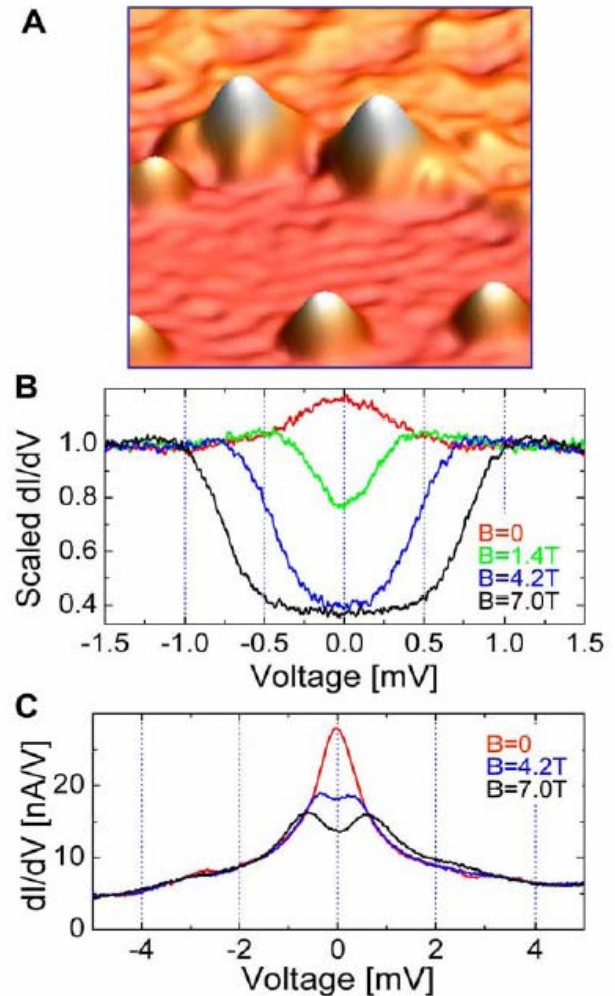
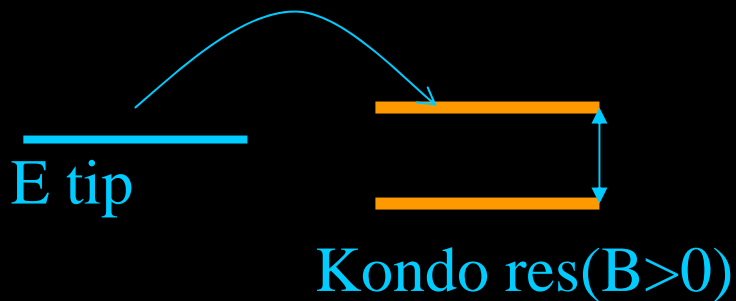


# Single Spin Flip Spectroscopy

Scienceexpress

## Single-Atom Spin-Flip Spectroscopy

A. J. Heinrich,\* J. A. Gupta, C. P. Lutz, D. M. Eigler



## *Case of distributed scatterers: collective modes and McMillan Rowell inversion for STM IETS*

- We will now look at the case where scattering is everywhere in a sample  
e.g. phonon, spin modes in high  $T_c$  materials
- Can we see nontrivial inelastic features in IETS,  $\frac{d^2 I}{dV^2}(r, eV)$  ?
- What can we say about the possible glue:  $\alpha^2 F(q, \omega)$

# IETS (Inelastic Electron Tunneling Spectroscopy) & Superconductivity

Eliashberg, G. M. Interactions between electrons and lattice vibrations in a superconductor. *Zh. Eksp. Teor. Fiz.* **38**, 966–976 (1960); *Sov. Phys. JETP* **11**, 696–702 (1960).

Theory: Expt.

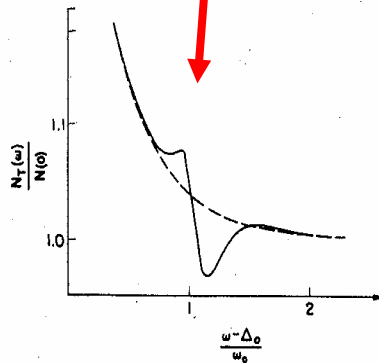
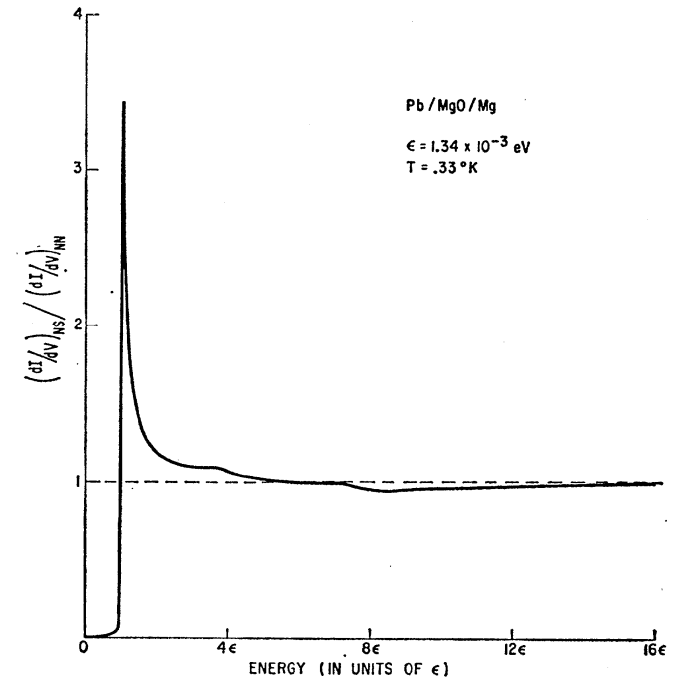


Fig. 38. Normalized tunneling density of states  $N_T(\omega)/N(0)$  (solid) compared with the BCS form (dashed) for the case of a phonon density of states with peak at  $\omega_0$  (see Fig. 34).

D. J. Scalapino, ch. 10, *SUPERCONDUCTIVITY*, ed. Parks, 1969.

Key observable is  $d^2I/dV^2$



Glaever et al., *Phys. Rev.* **126** No. 3, p941, 1962.

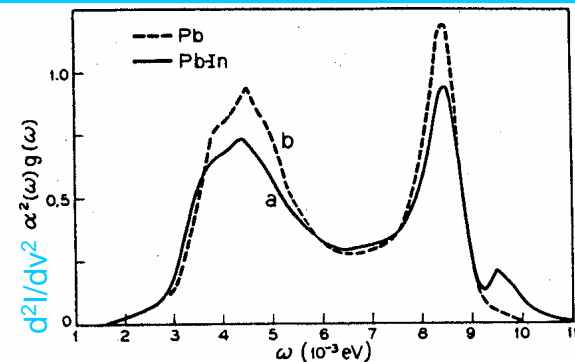


Fig. 36.  $\alpha^2 F(\omega)$  for  $\text{Pb}_{0.97}\text{In}_{0.03}$  from (13) compared with  $\alpha^2 F(\omega)$  for Pb.

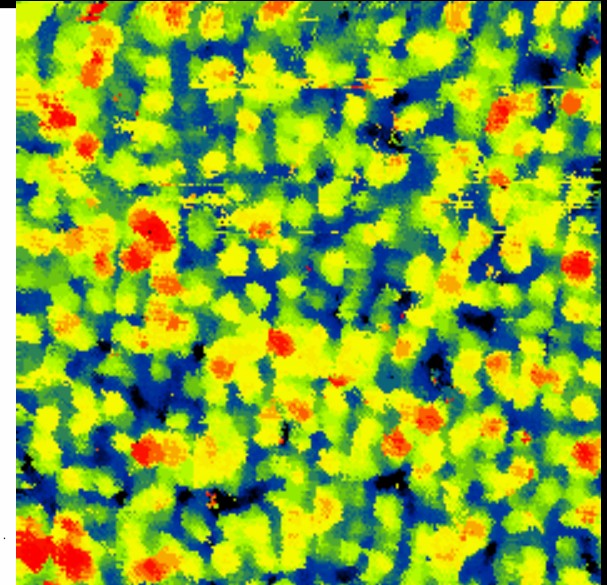
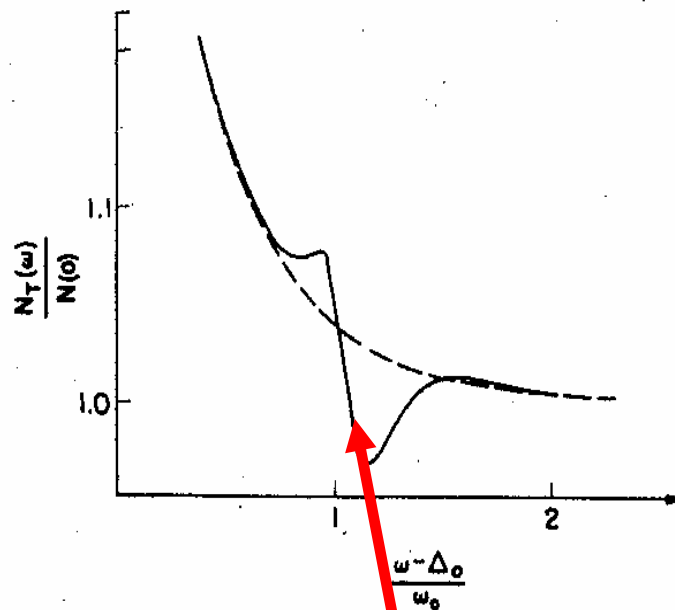


Fig. 38. Normalized tunneling density of states  $N_T(\omega)/N(0)$  (solid) compared with the BCS form (dashed) for the case of a phonon density of states with peak at  $\omega_0$  (see Fig. 34).

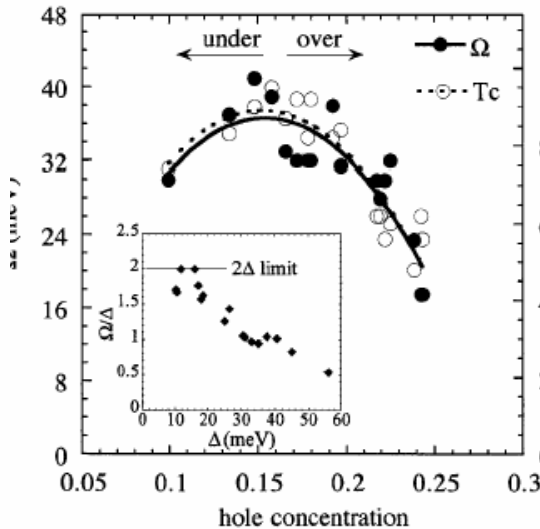
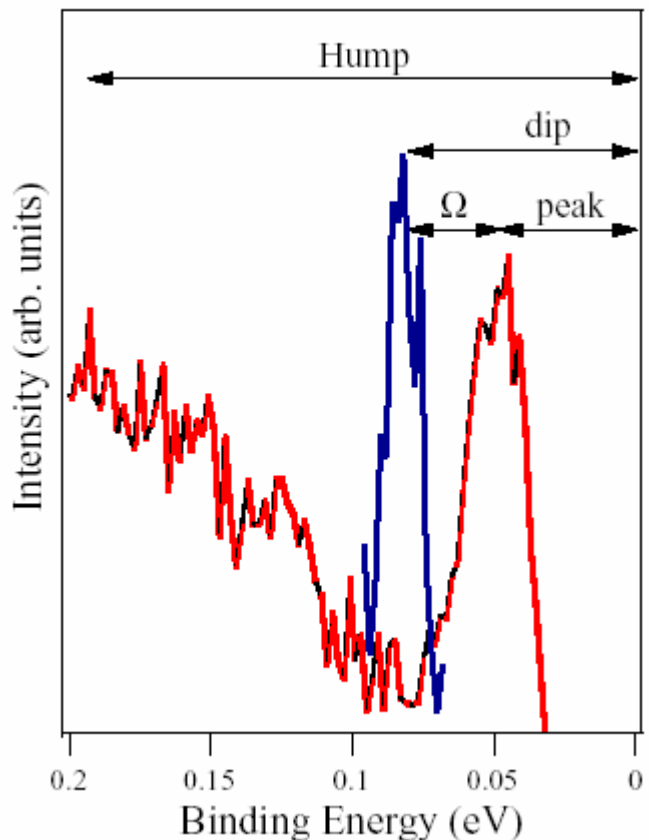
Remember !!!

# Previous Tunneling work

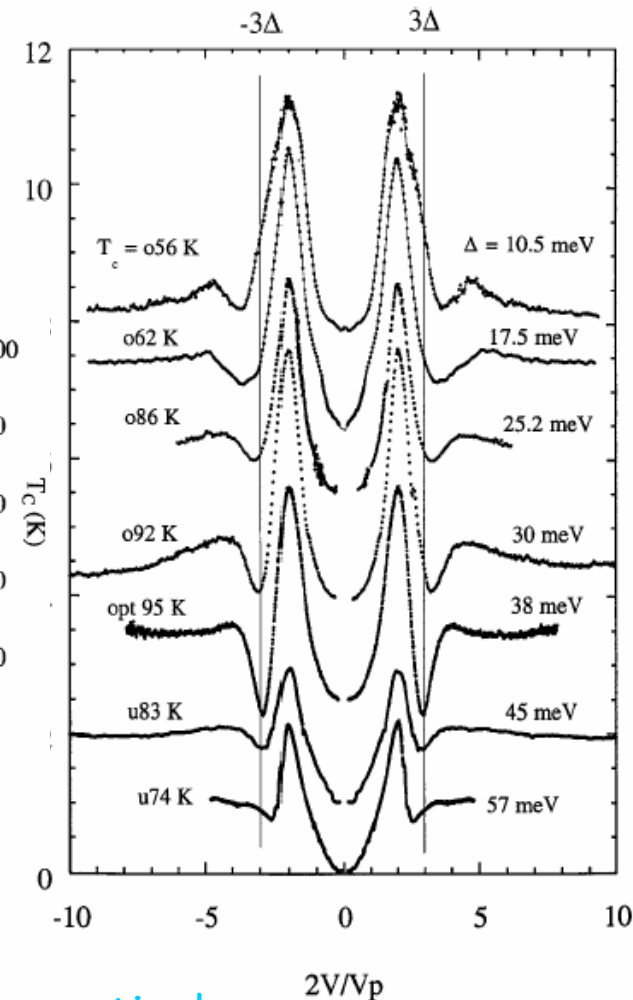
## Correlation of Tunneling Spectra in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ with the Resonance Spin Excitation

J. F. Zasadzinski,<sup>1,2</sup> L. Ozyuzer,<sup>2,3</sup> N. Miyakawa,<sup>4</sup> K. E. Gray,<sup>2</sup> D. G. Hinks,<sup>2</sup> and C. Kendziora<sup>5</sup>

M. Norman *et al*, PRL., 79, 3506 (1997)

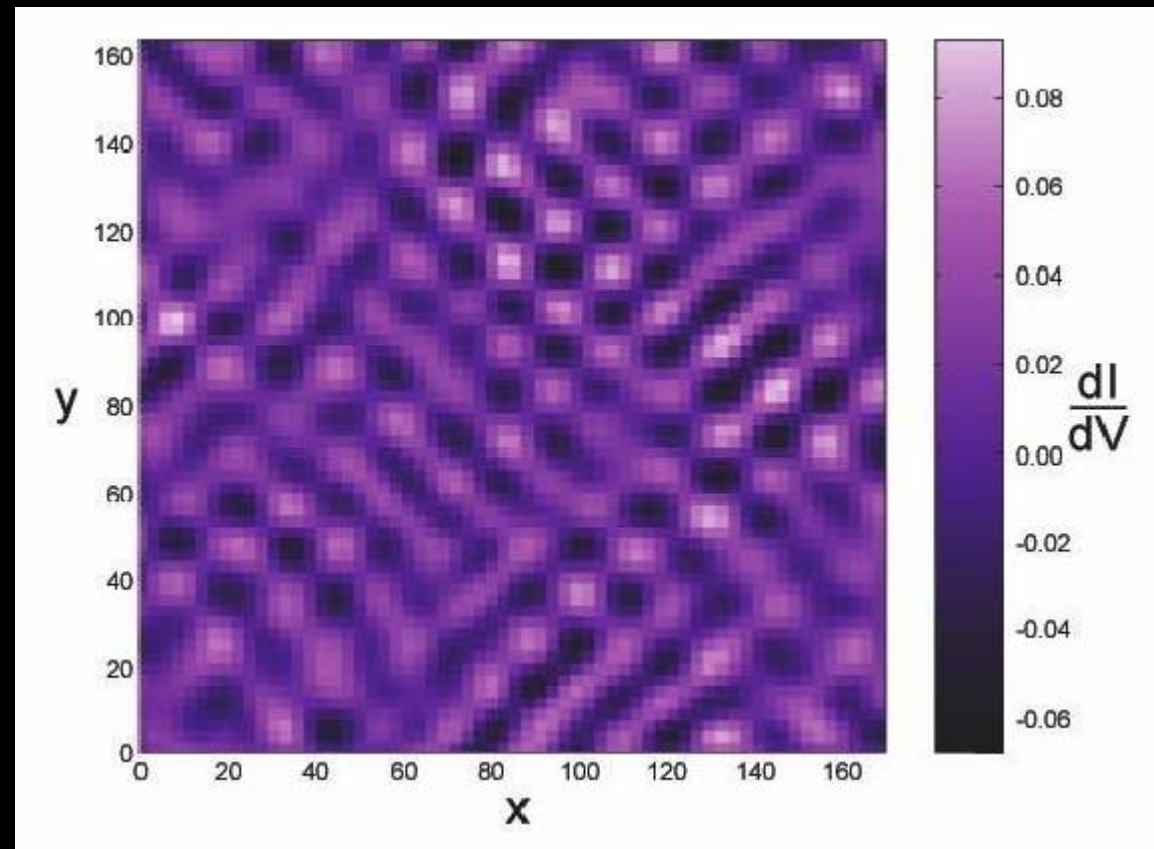


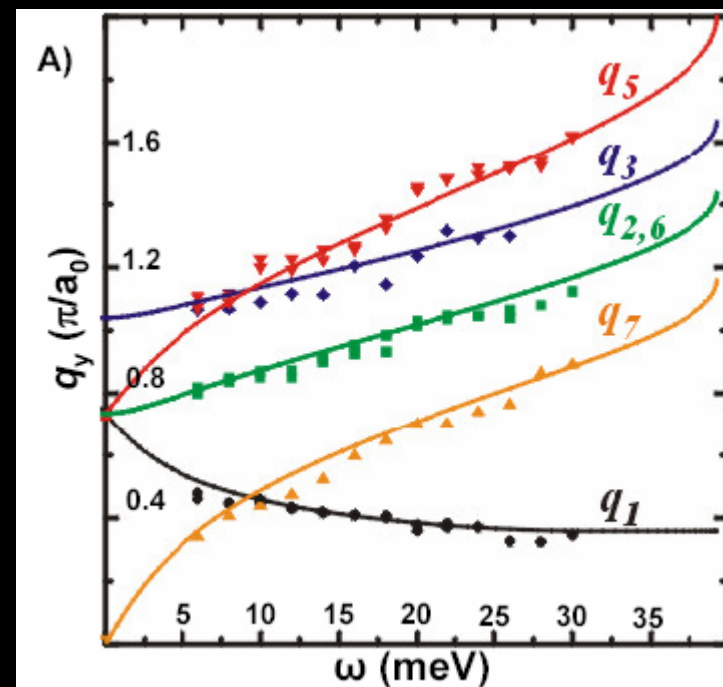
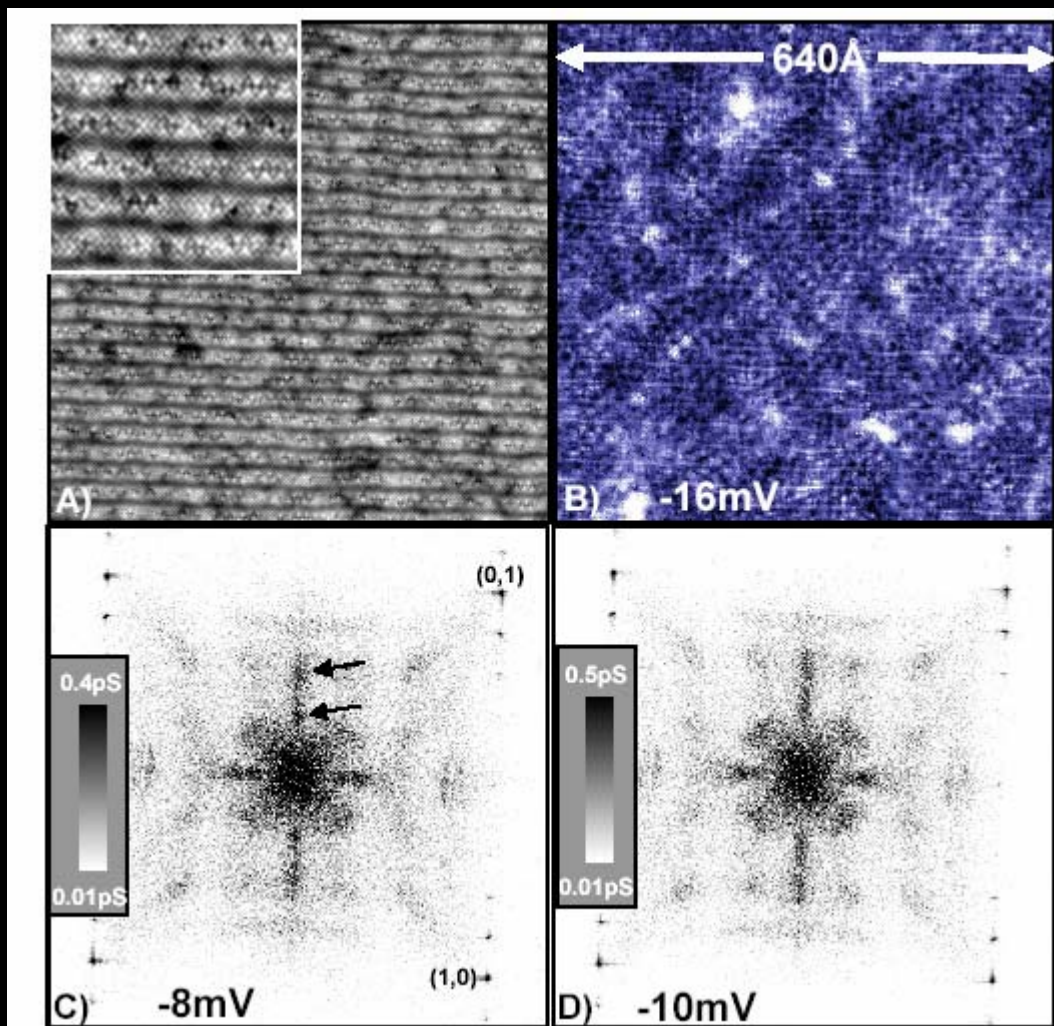
$$\alpha^2 F(\omega)$$



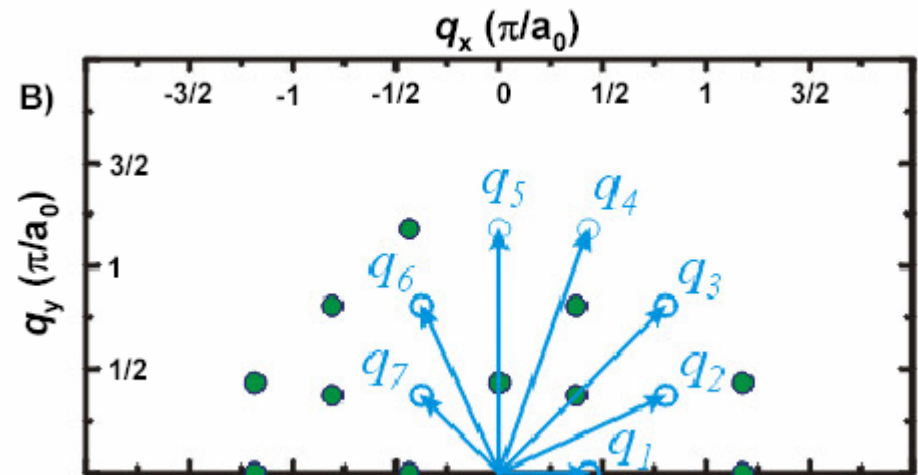
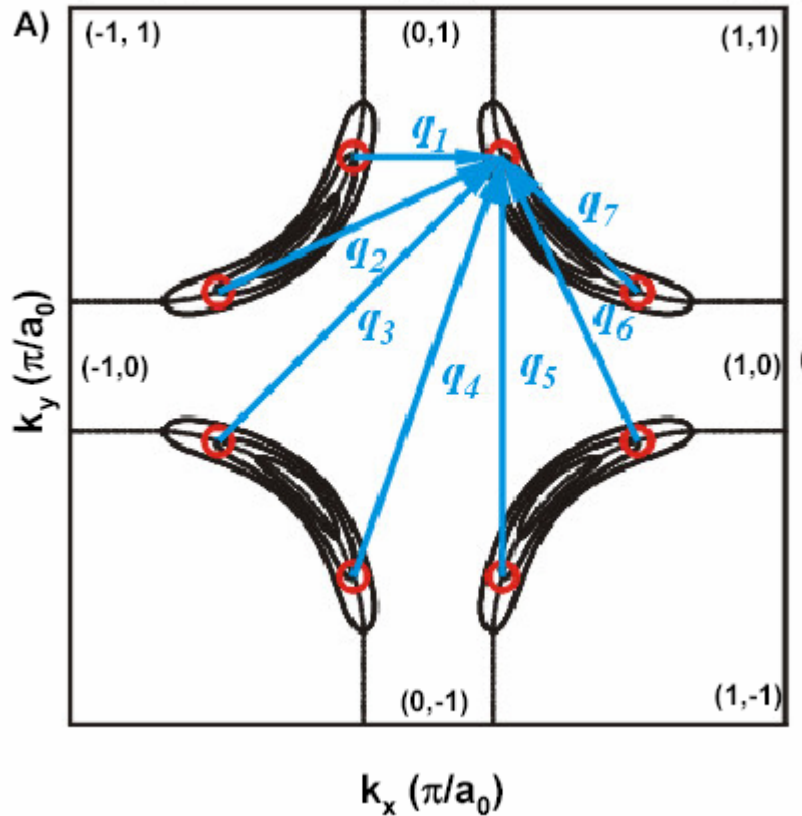
# *STM modulation*

STM, Howald et al., cond-mat/0201546

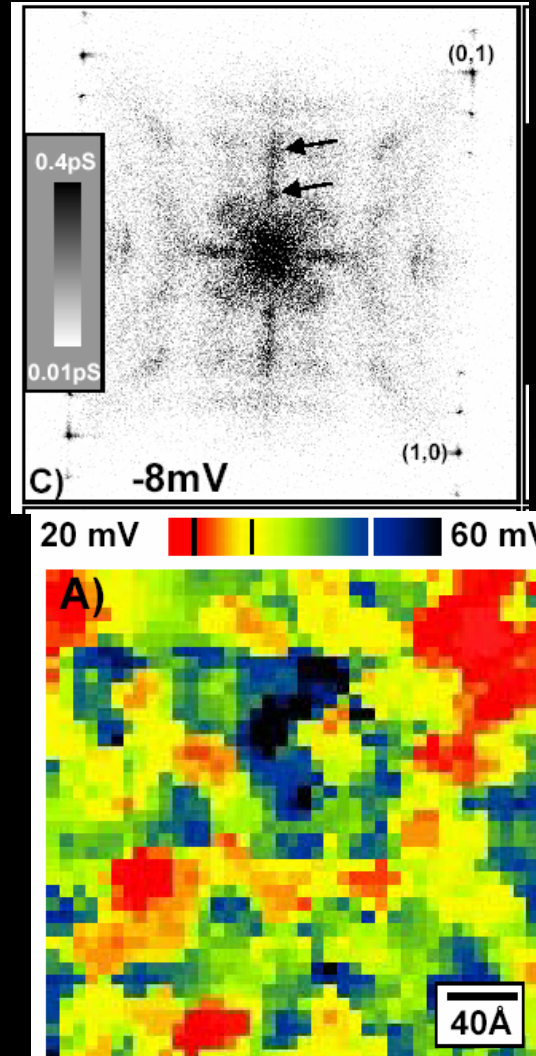
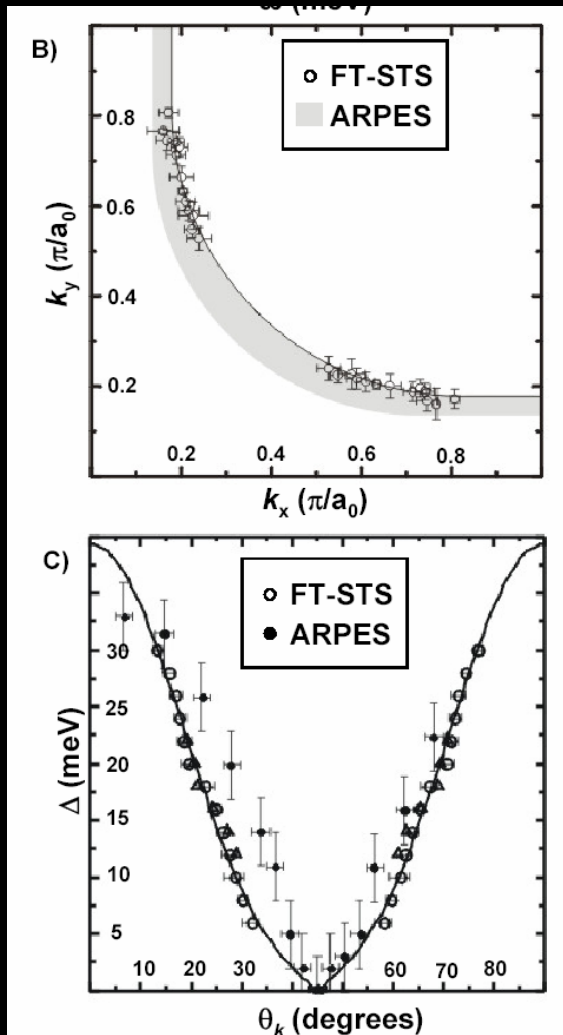




# *Davis et al STM results how we can get $k$ -space info*



# *Established connection of STM spectra to ARPES data*



Hoffman, McElroy  
et. al., Nature, 2003

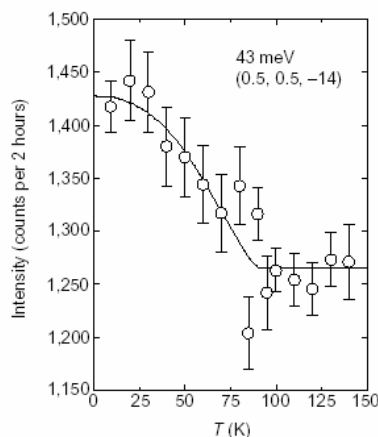
Can one make similar  
connection to Neutron  
42 meV mode?

One can see some  
boconic excitation.

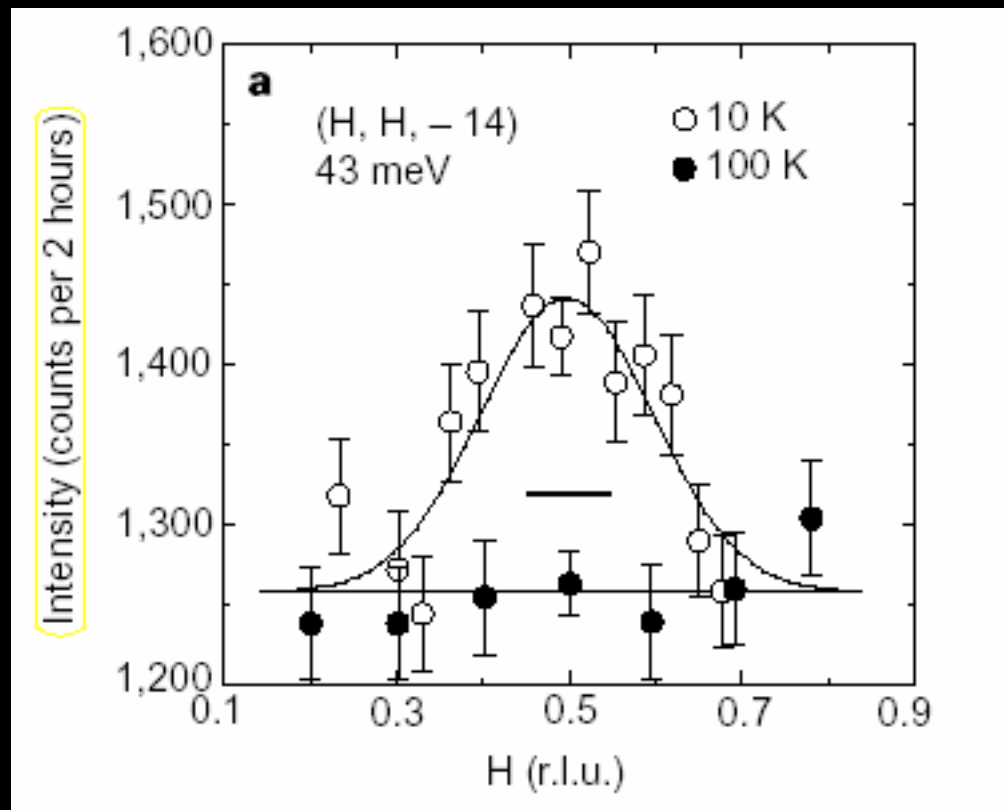
# INS on BSCCO

Fong et al., Nature, '99

- Origin of collective mode
- $5 T_c = E$  -energy of resonance is a rule
- Intensity of the mode scales as  $(T - T_c)^2$



**Figure 3** Temperature dependence of the neutron intensity at energy 43 meV and wavevector  $\mathbf{Q} = (0.5, 0.5, -14)$ . The intensity falls to background level above  $T_c = 91$  K (Fig. 1). The line is a guide to the eye.



# *70 meV kink and e-ph coupling in high- $T_c$ materials*

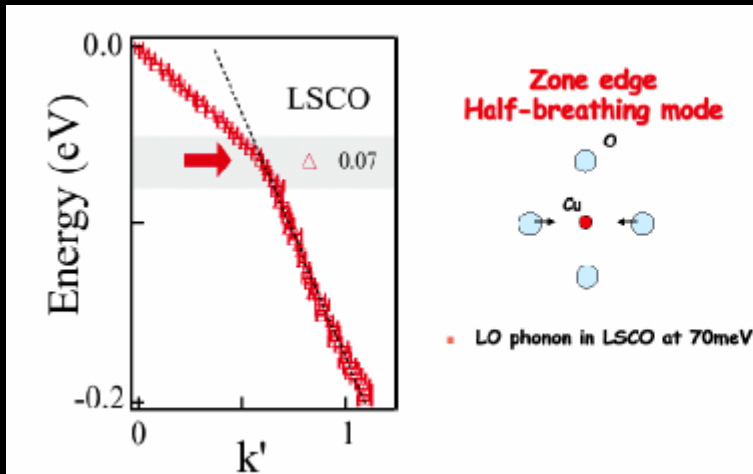


Figure 14.

ARPES derived dispersion from 10% doped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  system. A sudden change of dispersion is seen. The red arrow (and the gray bar) illustrates the energy where in plane phonon (as shown in the right panel) softening is observed.

Z.X. Shen,  
 A. Lanzara '03

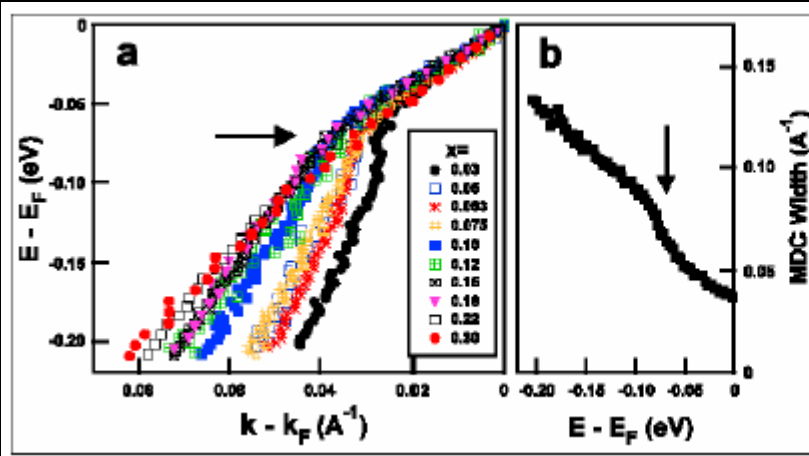


Figure 15.

Left panel, dispersion of LSCO from  $x = 0.03$  to  $x = 0.3$ . Right panel, scattering rate (reflected in the width of the so-called momentum distribution curve) for  $x = 0.63$  sample.

## *Model and formalism*

$$\mathcal{H} = \mathcal{H}_{BCS} + \mathcal{H}_{cp} + \mathcal{H}_{imp}$$

$$\mathcal{H}_{BCS} = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\Delta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\uparrow}^{\dagger} + \Delta_{\mathbf{k}}^{*} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow})$$

$$\mathcal{H}_{cp} = g \sum_i \mathbf{S}_i \cdot \mathbf{s}_i$$

$$\mathcal{H}_{imp} = U_0 \sum_{\sigma} c_{0\sigma}^{\dagger} c_{0\sigma}$$

## *Model and formalism (cont'd)*

Bare GF:  $\hat{G}_0^{-1}(\mathbf{k}; i\omega_n) = \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & i\omega_n + \xi_{\mathbf{k}} \end{pmatrix} .$

Self energy:  $\hat{\Sigma}(\mathbf{k}; i\omega_n) = \frac{g^2 T}{8N} \sum_{\mathbf{q}} \sum_{\Omega_l} \chi(\mathbf{q}; i\Omega_l) \begin{pmatrix} 3G_{0,11} & G_{0,12} \\ G_{0,21} & 3G_{0,22} \end{pmatrix} (\mathbf{k} - \mathbf{q}; i(\omega_n - \Omega_l)) .$

Dressed GF:  $\underline{\hat{G}}_0^{-1}(\mathbf{k}; i\omega_n) = \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} - \Sigma_{11} & \Delta_{\mathbf{k}} - \Sigma_{12} \\ \Delta_{\mathbf{k}} - \Sigma_{21} & i\omega_n + \xi_{\mathbf{k}} - \Sigma_{22} \end{pmatrix} .$

## *Model and formalism (cont'd)*

Site-dependent GF (TMA) w/ imp:

$$\hat{G}(i, j; E) = \underline{\hat{G}}_0(i, j; E) + \underline{\hat{G}}_0(i, 0; E) \hat{T}(E) \underline{\hat{G}}_0(0, j; E)$$

$$\hat{T}^{-1} = U_0^{-1} \sigma_3 - \underline{\hat{g}}_0, \quad \underline{\hat{g}}_0(i\omega_n) = \underline{\hat{G}}_0(i, i; i\omega_n)$$

$$\text{LDOS: } \rho_i(E) = -\frac{2}{\pi} \text{Im} G_{11}(i, i; E + i\gamma).$$

$$\text{Band DOS } (U_0 = 0): \rho(E) = \sum_{\mathbf{k}} A_{\mathbf{k}}(E). \quad A_{\mathbf{k}}(E) = -\frac{2}{\pi} \text{Im} \underline{G}_{0,11}(\mathbf{k}; E + i\gamma).$$

## *Numerical results and discussions*

Parameter values:  $t = 1.0$ ,  $t' = -0.2$  [ $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$ ]

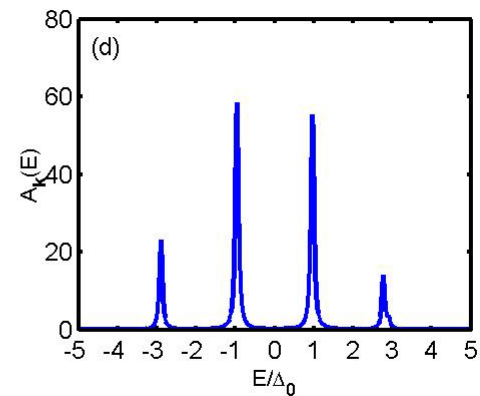
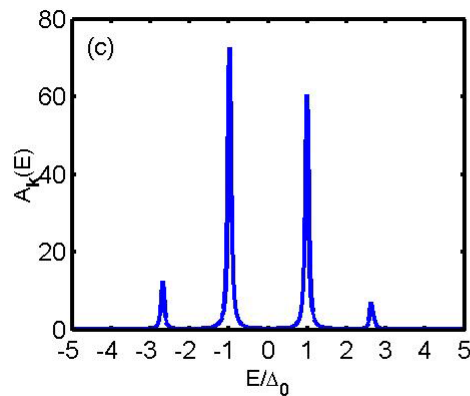
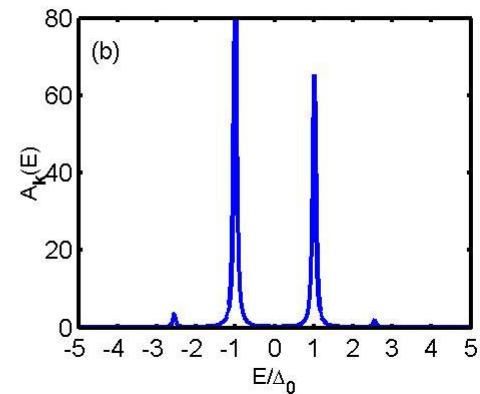
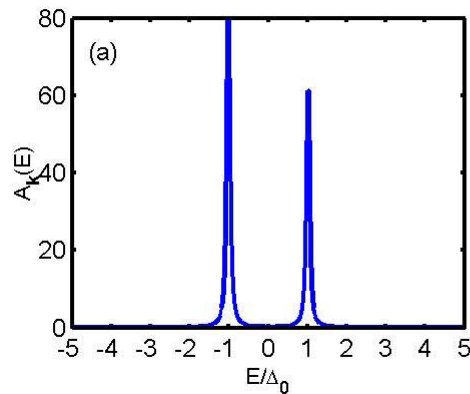
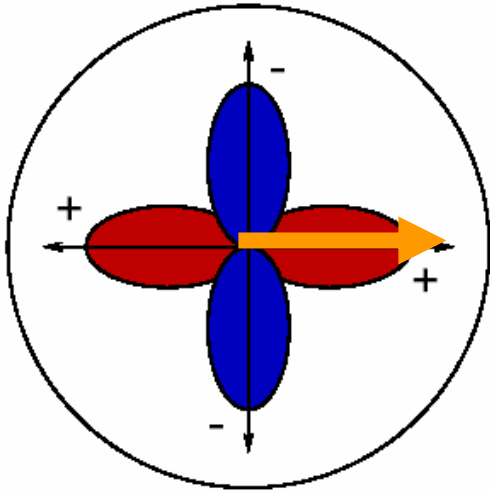
$$\Delta_0 = 0.1 \quad [\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y)]$$

Ansatz for mode:

$$\chi(\mathbf{q}; i\Omega_l) = -\frac{N\delta_{\mathbf{q},\mathbf{Q}}}{2} \left[ \frac{1}{i\Omega_l - \Omega_0} - \frac{1}{i\Omega_l + \Omega_0} \right]$$

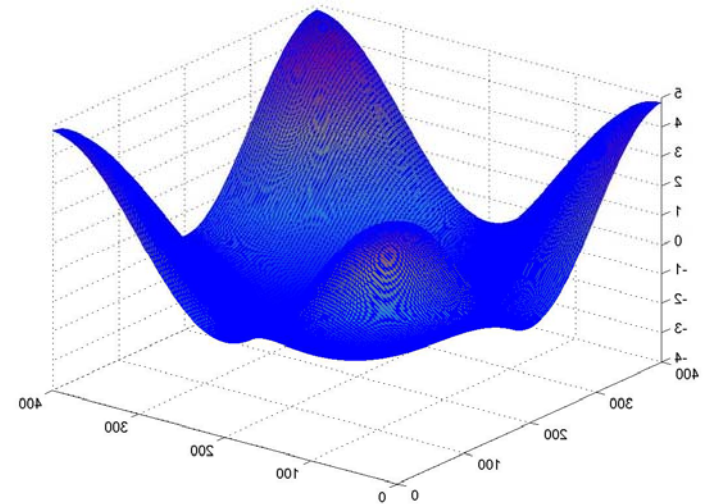
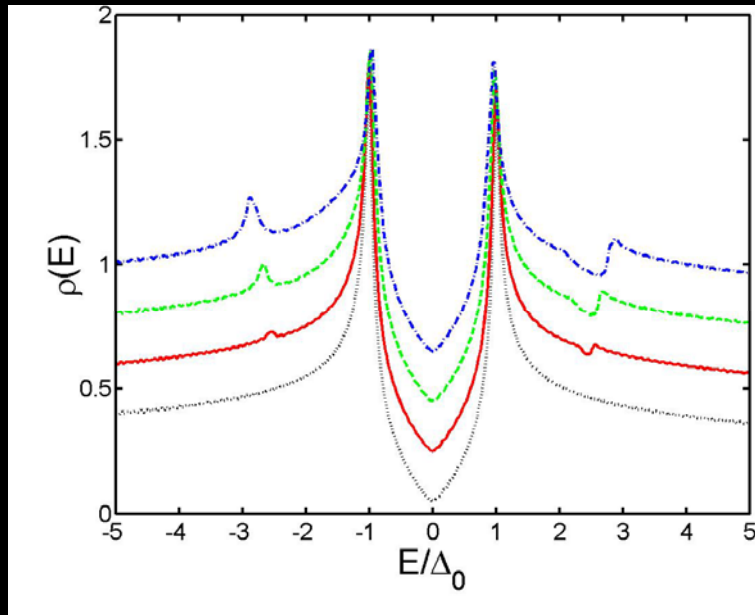
$\mathbf{Q} = (\pi, \pi)$  and  $\Omega_0 = 0.15$ .

# *Spectral function at M point*



$$g/\Delta_0 = 0, 1, 2, 3$$

# *Band density of states*

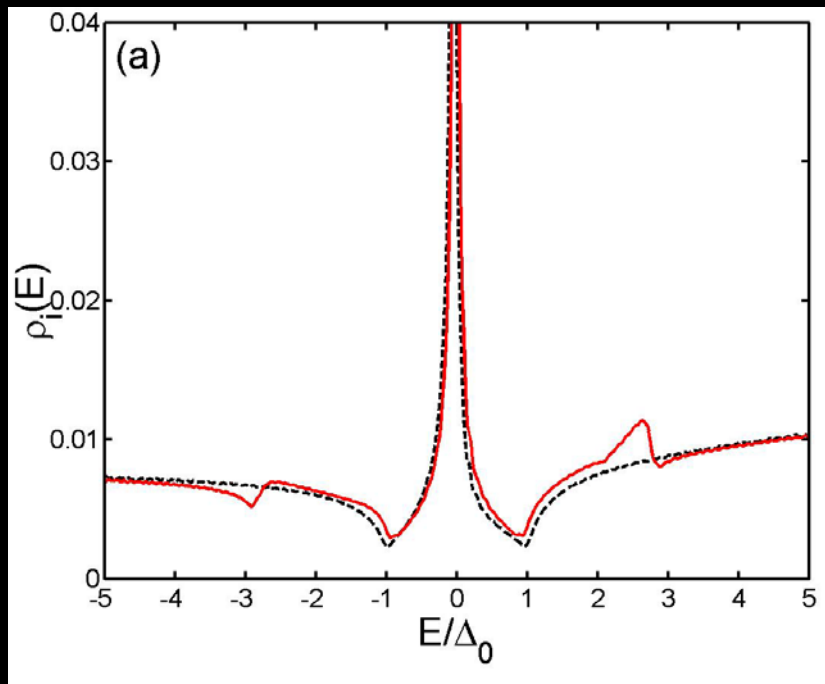


Translationally invariant image

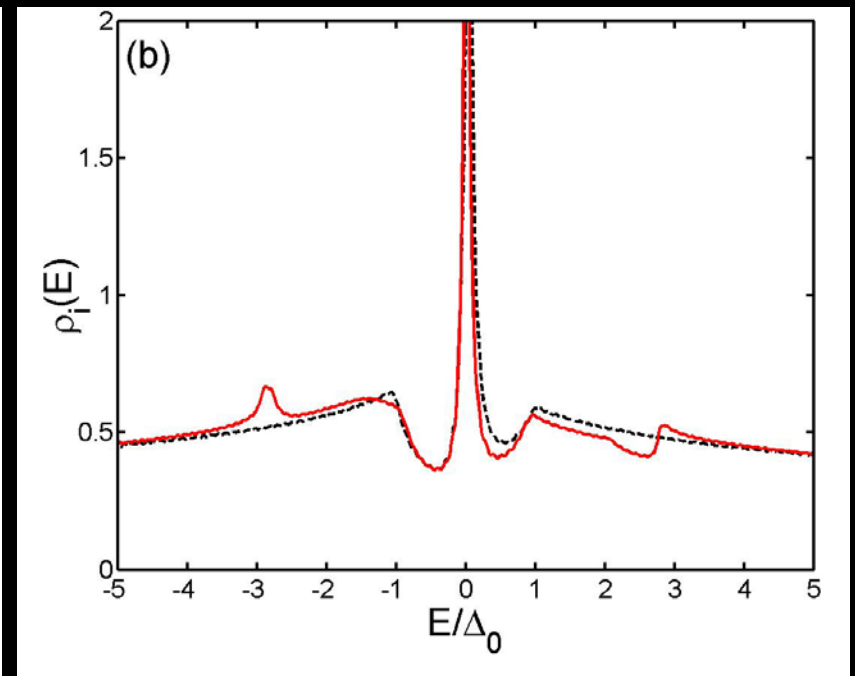
$\epsilon_{\mathbf{k}}$

# *Local density of states*

$$U_0 = 100\Delta_0 \quad g = 3\Delta_0$$

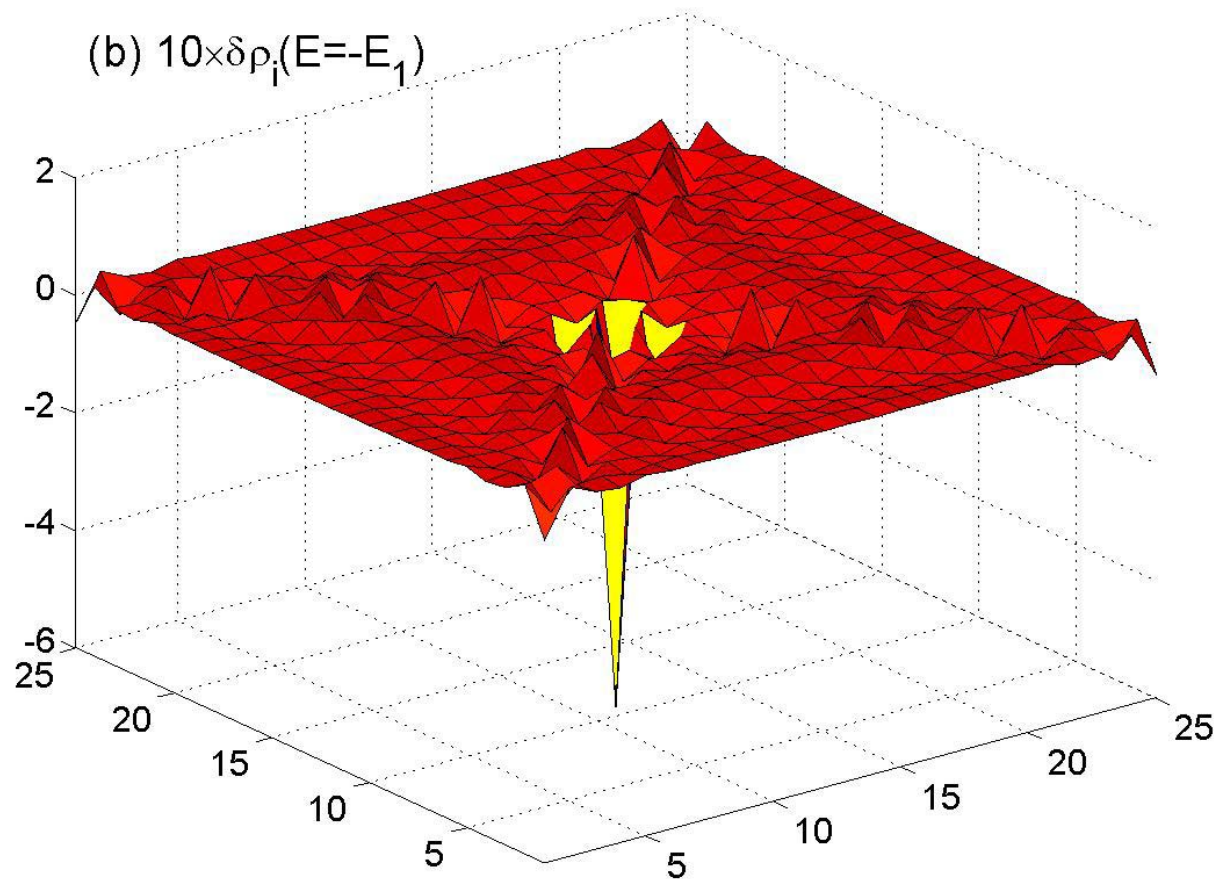


$$\mathbf{r}_i = (0, 0)$$



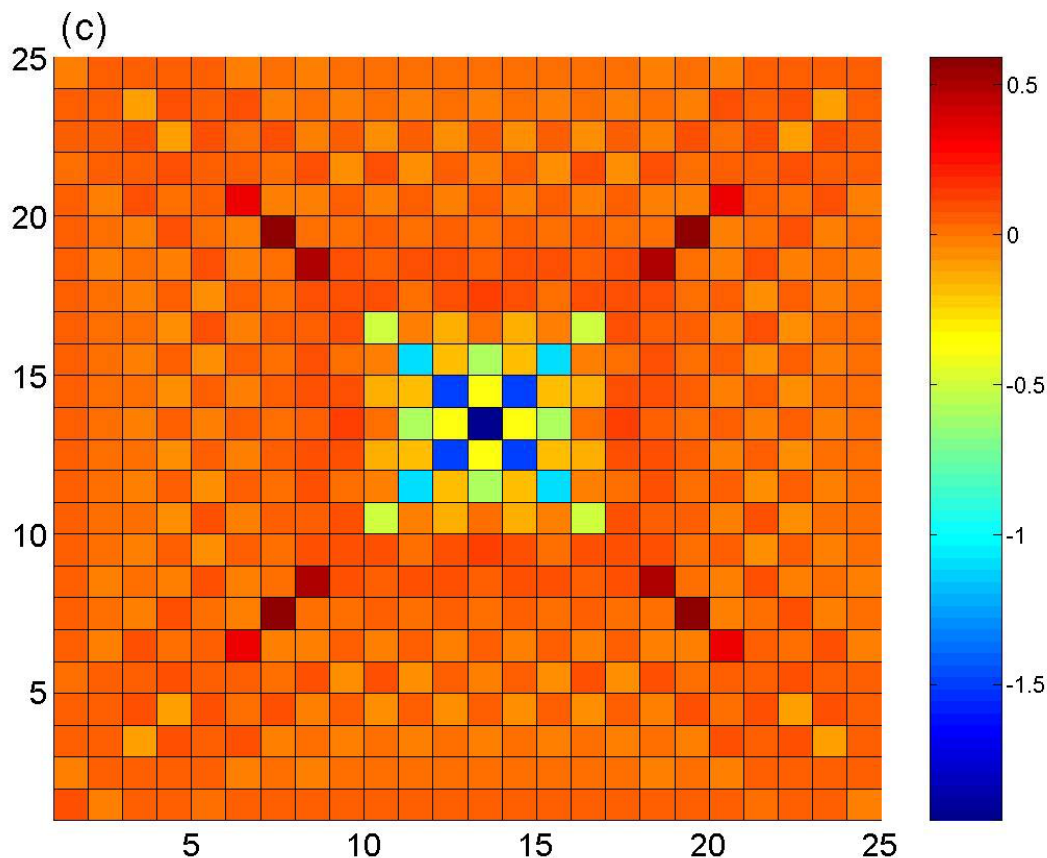
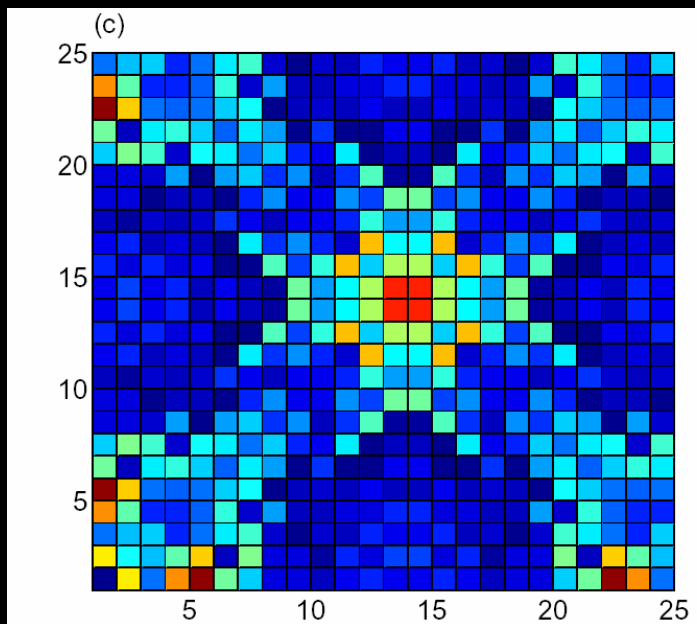
$$\mathbf{r}_i = (1, 0)$$

# *LDOS imaging at $E=-E_1$ $(g/\Delta_0=3)$*



# *LDOS imaging at $E=-E_1$ (Contrast)*

Scattering from the local  
 center produces the modulation  
 at Q



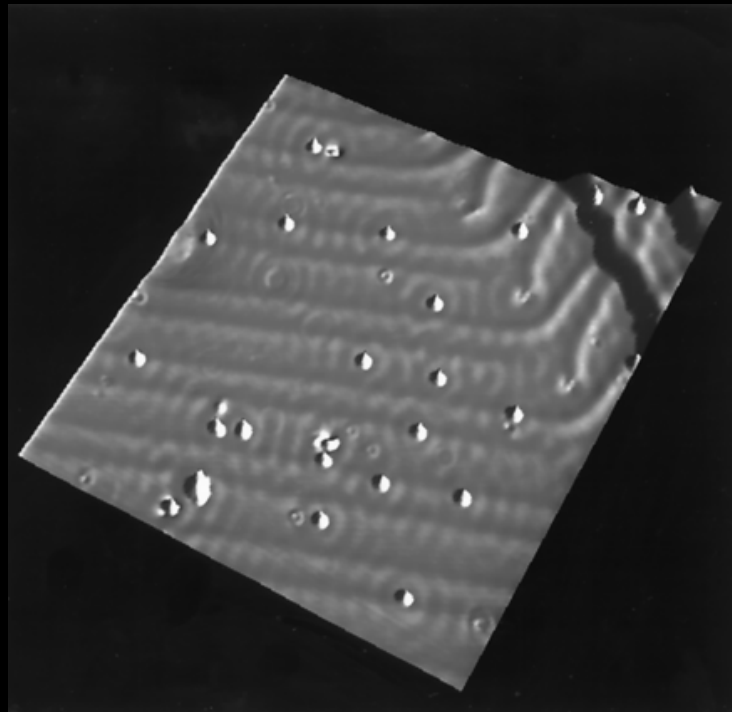
## *Local DOS math and examples*

$$\delta N(r, \omega) = \int dr' U(r') G(r, r', \omega) G(r', r, \omega)$$

$$\delta N(p, \omega) = U(p) \Lambda(p, \omega)$$

$$\Lambda(p, \omega) = \sum_q G(p+q) G(q)$$

M. Crommie  
 Charge Friedel  
 oscillations on Cu  
 surface

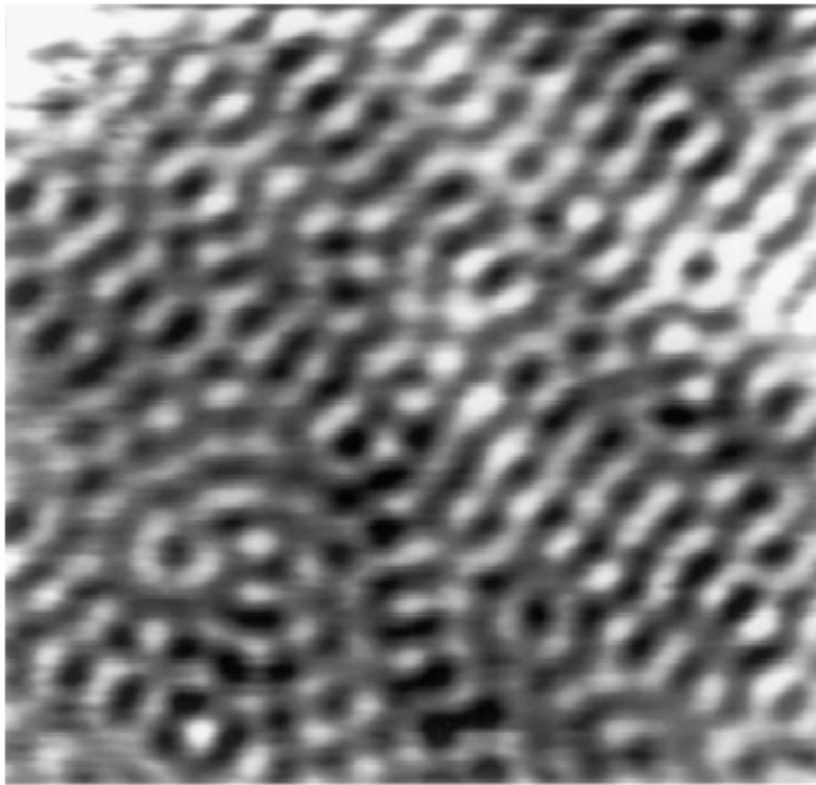


Fourier transform  
 gives  $2k_F$  Fermi Surface

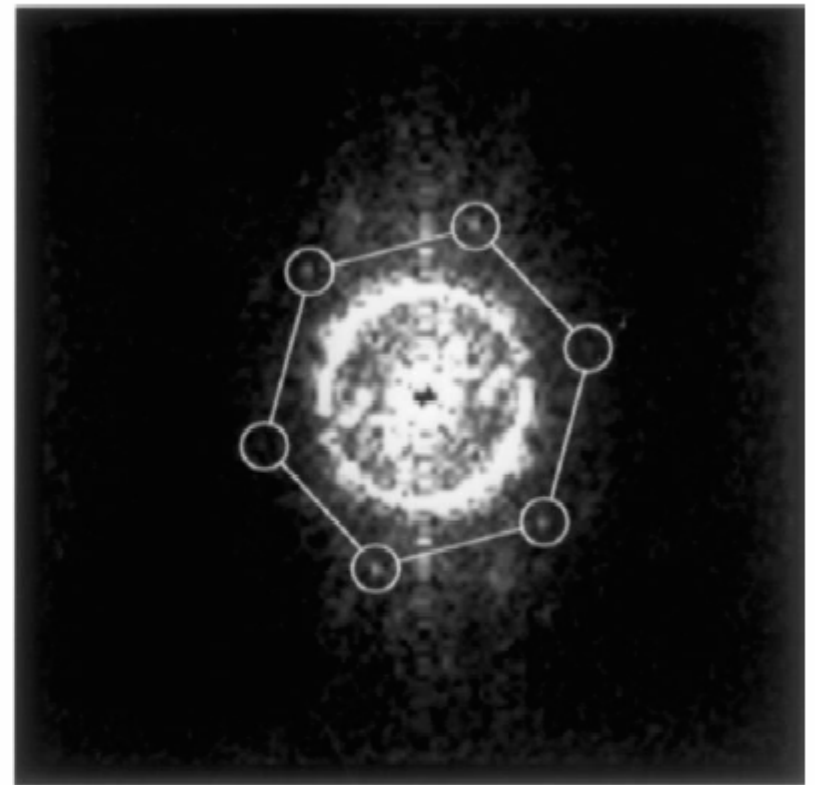
# Fourier Transform–STM: determining the surface Fermi contour

L. Petersen<sup>a,\*</sup>, Ph. Hofmann<sup>b</sup>, E.W. Plummer<sup>c,d</sup>, F. Besenbacher<sup>a</sup>

Journal of Electron Spectroscopy and Related Phenomena 109 (2000) 97–115

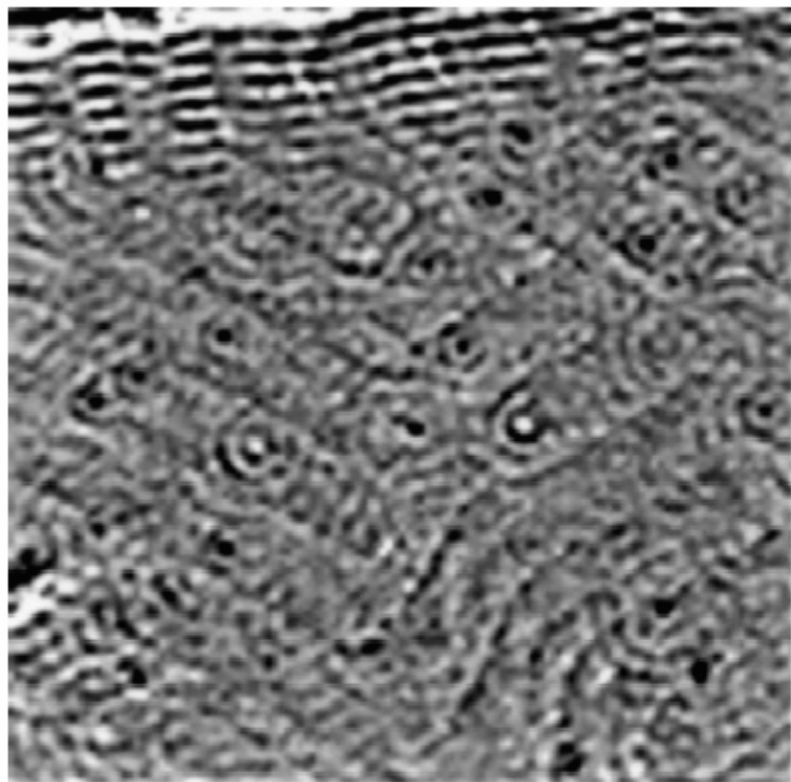


(a)

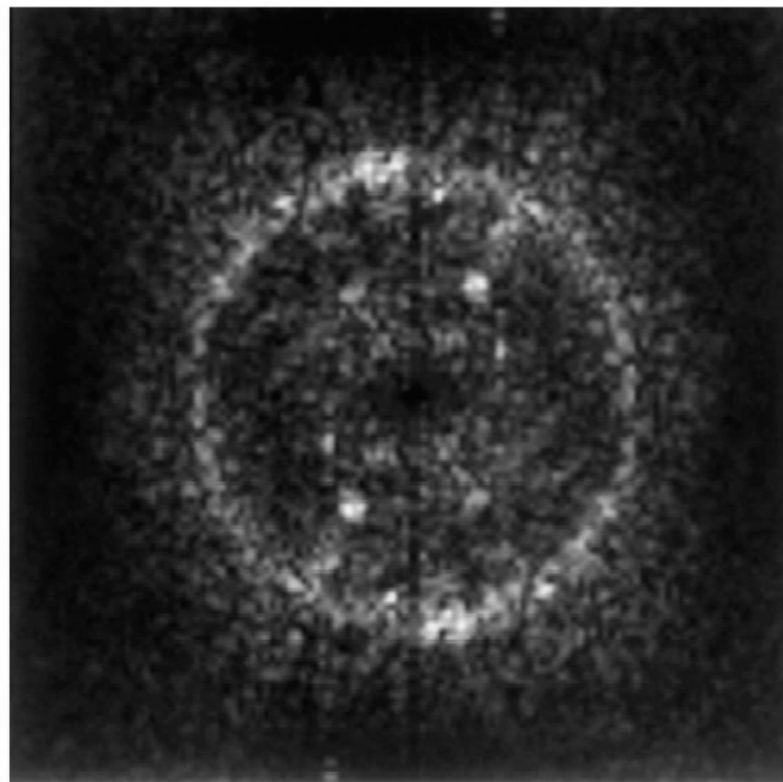


(b)

Fig. 2. (a) Constant-current STM image of the Be(0001) surface.  $V = 2.7$  mV,  $I = 2.9$  nA,  $T = 150$  K,  $55 \times 55 \text{ \AA}^2$ . (b) The 2-D Fourier transform (power spectrum) of (a). The hexagon serves to guide the eye with respect to the six lattice spots (see text).

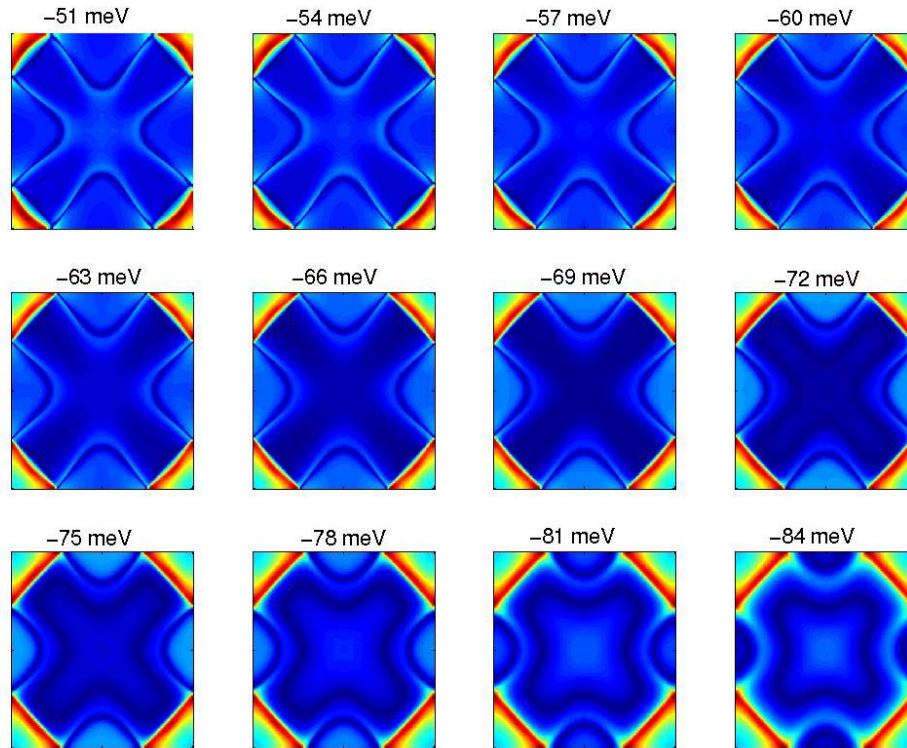


(a)



(b)

Fig. 6. (a) Constant-current STM image of standing waves on Au(111) emanating from point defects of unknown chemical identity and a step edge located in the top of the image. The image has been slightly processed to enhance the standing waves ( $V = 1.2$  mV,  $I = 1.5$  nA,  $T = 130$  K,  $609 \times 630 \text{ \AA}^2$ ). (b) Power spectrum of the Fourier transform of (a). The dots positioned in a (vague) cross inside the Fermi contour circle represent topographical information about the reconstruction.



$$\omega_{B_{1g}} = 36 \text{ meV}$$

$$\omega_{br} = 72 \text{ meV}$$

$$\phi_x = \frac{-i}{\mathcal{N}_{\mathbf{k}}} [\xi_{\mathbf{k}} t_{x,\mathbf{k}} - t_{xy,\mathbf{k}} t_{y,\mathbf{k}}],$$

$$\phi_y = \frac{i}{\mathcal{N}_{\mathbf{k}}} [\xi_{\mathbf{k}} t_{y,\mathbf{k}} - t_{xy,\mathbf{k}} t_{x,\mathbf{k}}],$$

$$\phi_b = \frac{1}{\mathcal{N}_{\mathbf{k}}} [\xi_{\mathbf{k}}^2 - t_{xy,\mathbf{k}}^2],$$

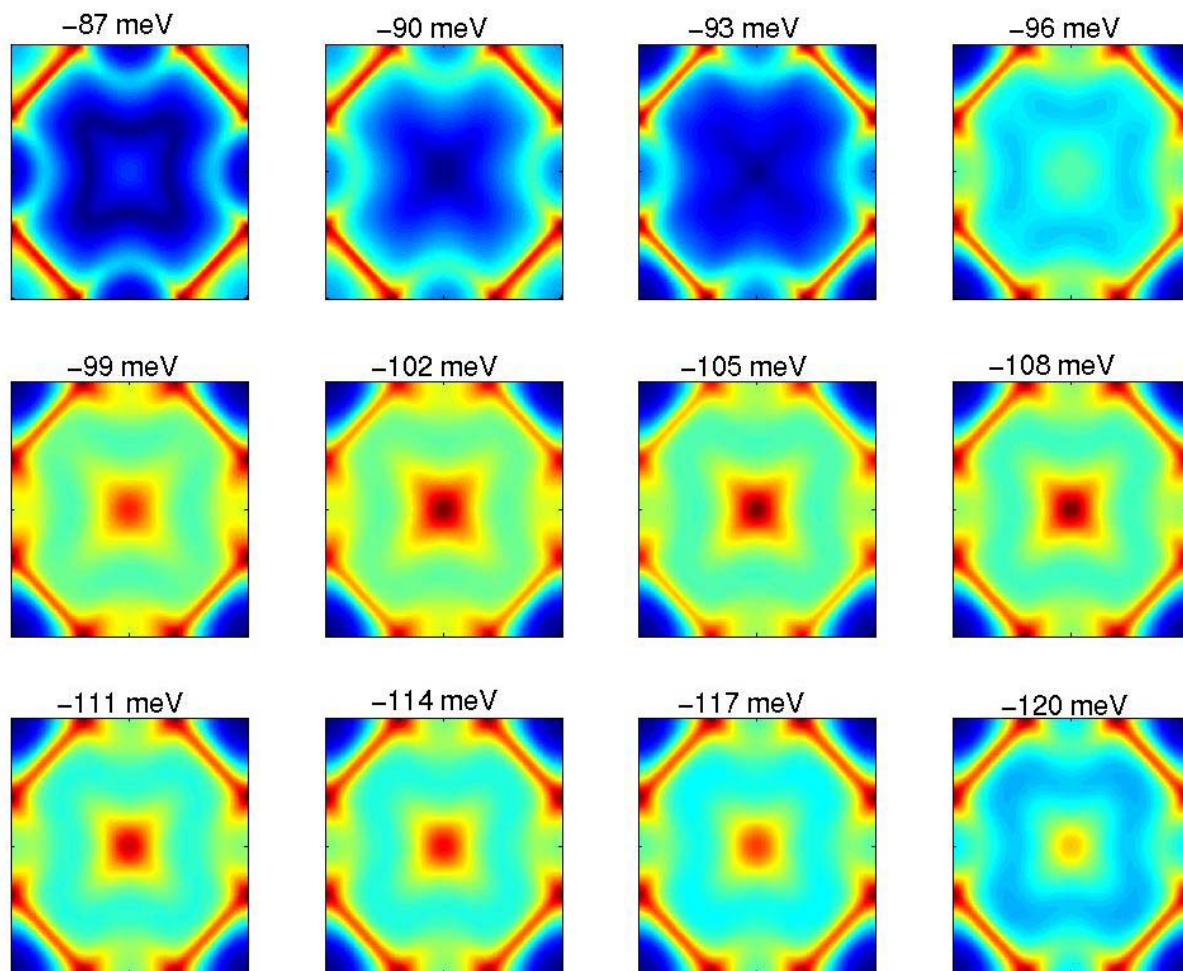
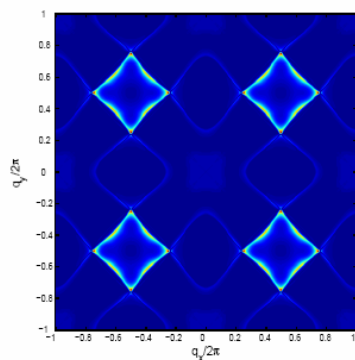
$$\mathcal{H}_{cl-ph} = \frac{1}{\sqrt{N_L}} \sum_{\sigma,\nu} \sum_{\mathbf{k},\mathbf{q}} g_{\nu}(\mathbf{k},\mathbf{q}) c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}\sigma} (b_{\nu\mathbf{q}} + b_{\nu,-\mathbf{q}}^{\dagger})$$

$$g_{B_{1g}}(\mathbf{k},\mathbf{q}) = \frac{g_{B_{1g},0}}{\sqrt{M(\mathbf{q})}} \{ \phi_x(\mathbf{k}) \phi_x(\mathbf{k} + \mathbf{q}) \cos(q_y/2) - \phi_y(\mathbf{k}) \phi_y(\mathbf{k} + \mathbf{q}) \cos(q_x/2) \},$$

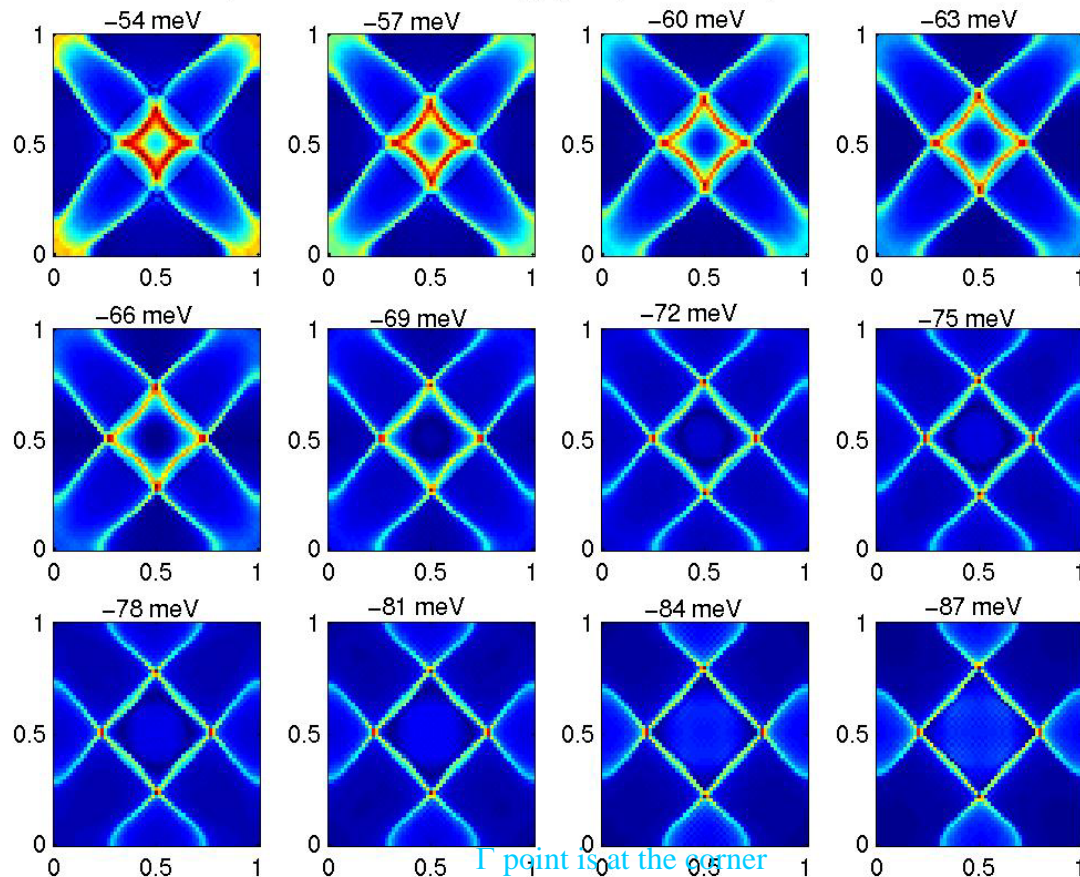
$$g_{br}(\mathbf{k},\mathbf{q}) = g_{br,0} \sum_{\alpha=x,y} \{ \phi_b(\mathbf{k} + \mathbf{q}) \phi_{\alpha}(\mathbf{k}) \cos[(k_{\alpha} + q_{\alpha})/2] - \phi_b(\mathbf{k}) \phi_{\alpha}(\mathbf{k} + \mathbf{q}) \cos(k_{\alpha}/2) \}.$$

# Energy evolution of FT spectrum in the presence of B1g and half-stretching breathing collective modes --- 2

No filter!  $\hbar$



FT spectrum evolution with energy (local phonon mode)

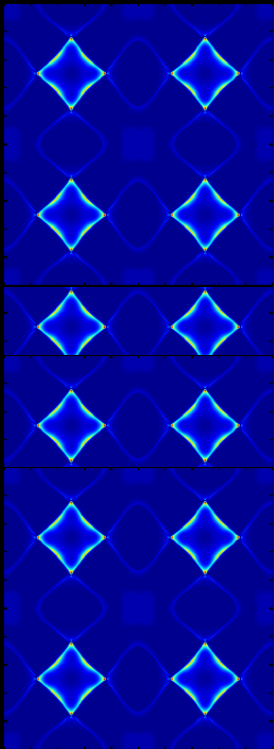


Note:  $k_x, k_y$  are in units of  $2\pi/a$

$$\mathcal{H}_{el-localph} = g_0 \sum_{\sigma} c_{0\sigma}^{\dagger} c_{0\sigma} (b_0 + b_0^{\dagger})$$

$$\Omega_0 = 36 \text{ meV}$$

# Experimental Algorithm



Measure a set of second-derivative images:

$$\frac{d^2 I}{dV^2}(\vec{r}, eV)$$

Fourier transform: second-derivative images:

$$\frac{d^2 I}{dV^2}(\vec{q}, eV)$$

Identify energies:

$$\Omega = eV - \Delta$$

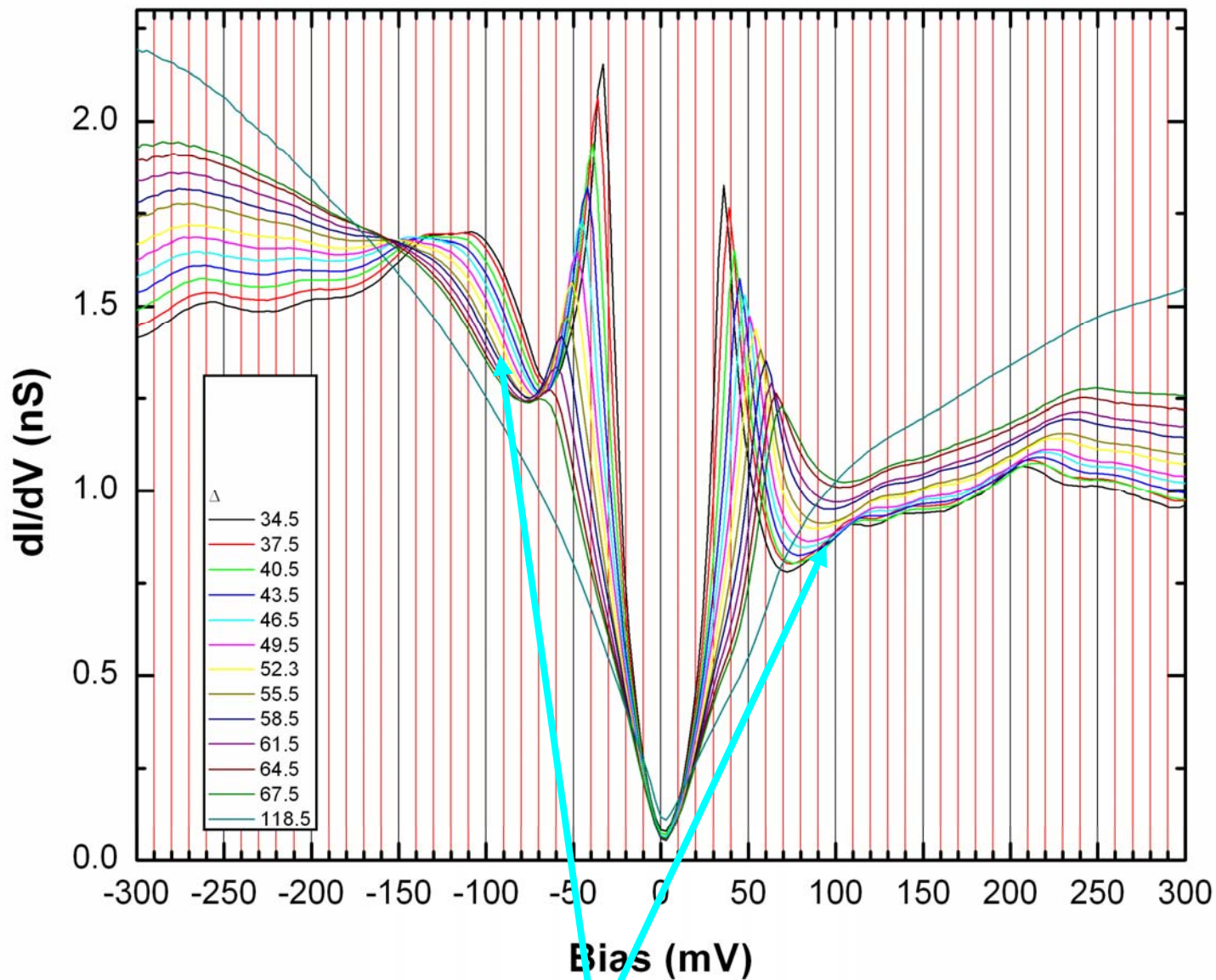
and  $\vec{q}$  –vectors:

$$\vec{q}(\Omega)$$

of peaks in  $\frac{d^2 I}{dV^2}(\vec{q}, eV)$  caused by

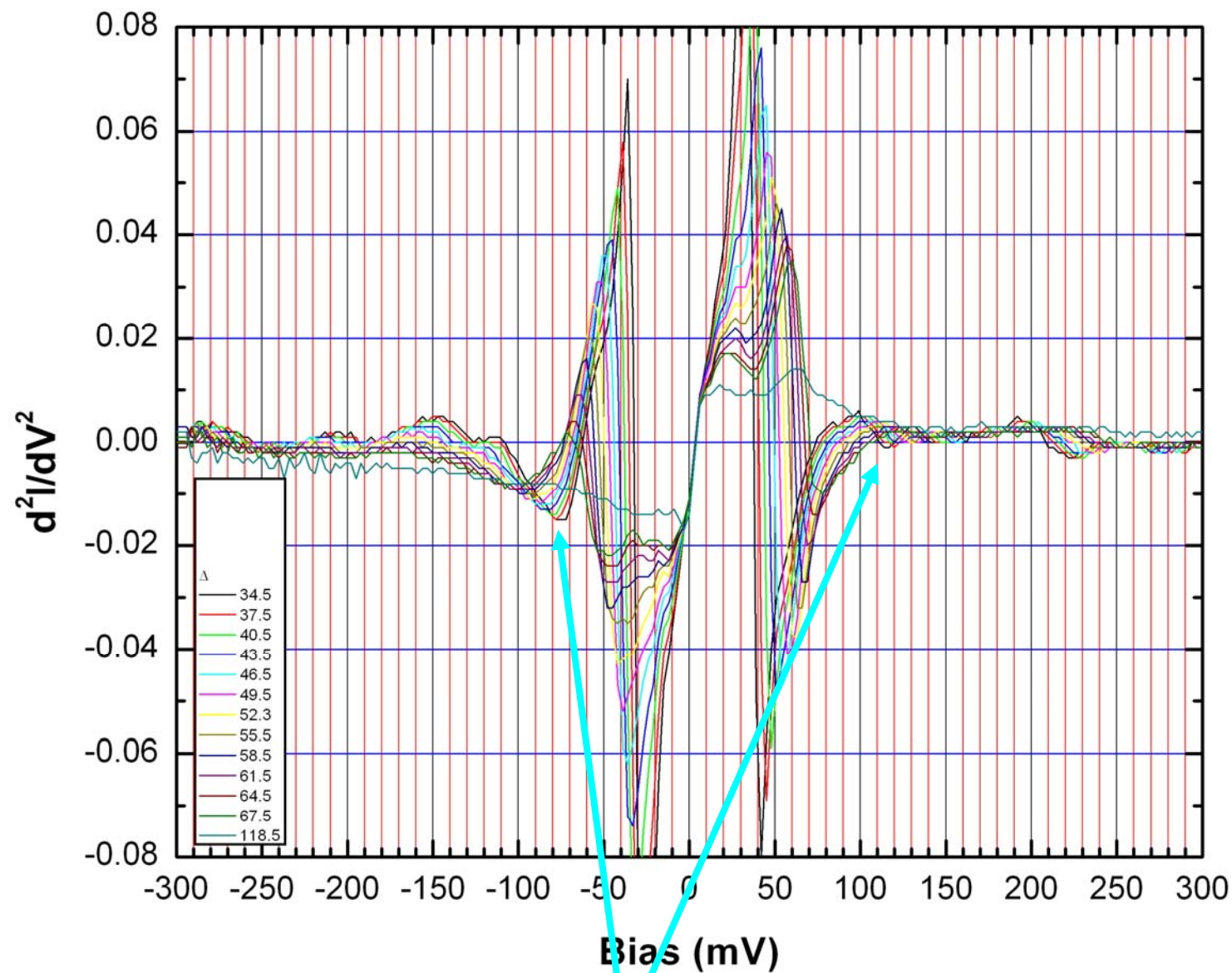
***Inelastic electron-boson interactions***

# $dI/dV$ of Bi-2212



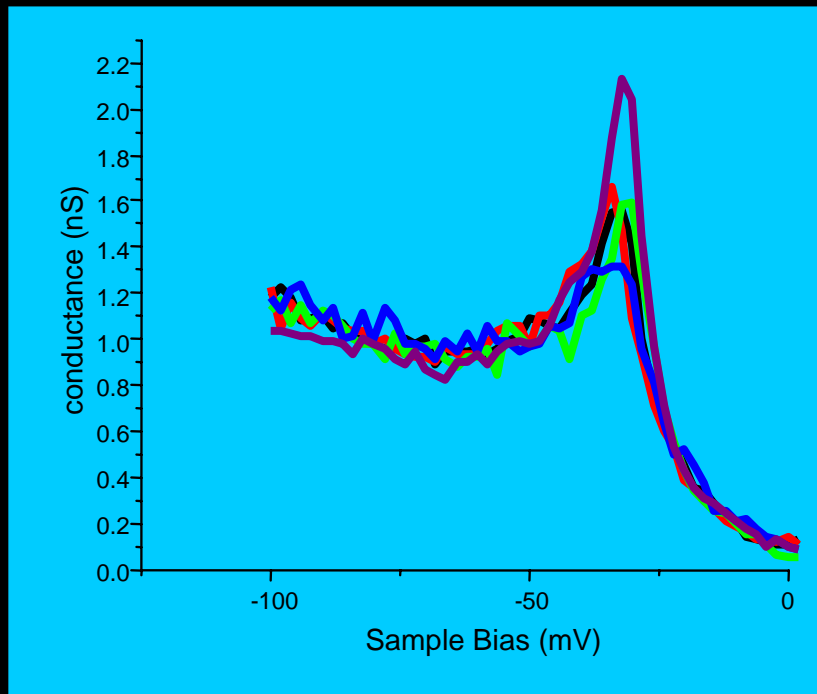
# $d^2I/dV^2$ of Bi-2212

Ine



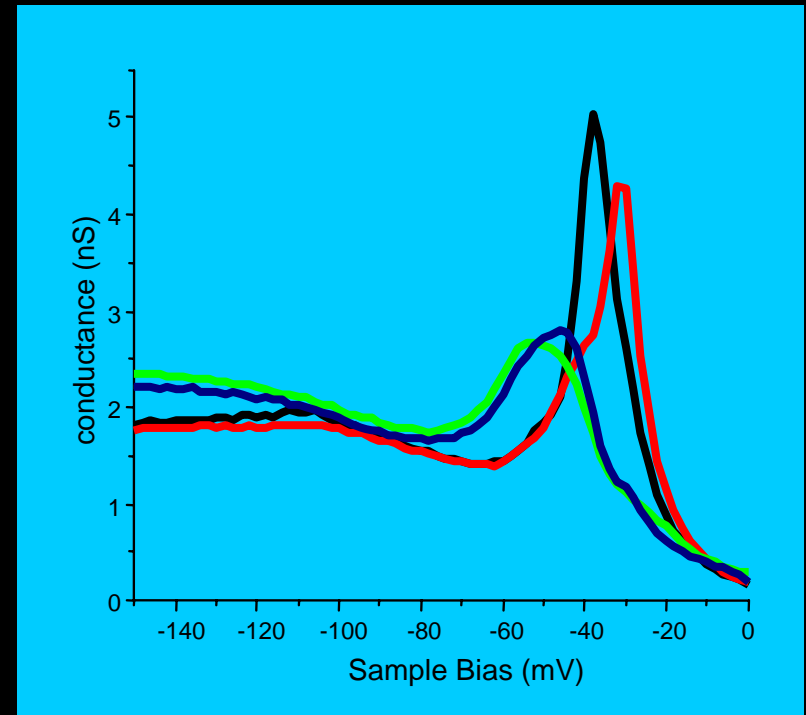
$$\Omega(\vec{r}) = E_{peak} - \Delta(\vec{r})$$

# Signal to noise increase of ~30 needed on a 256x256 grid of points



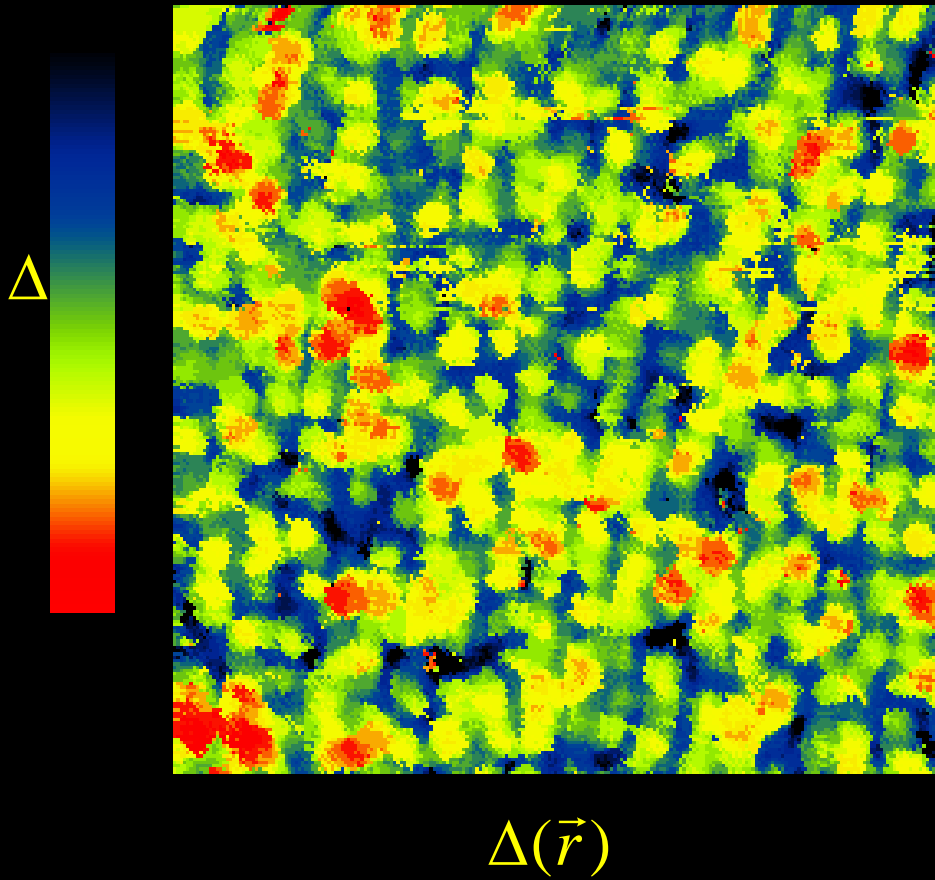
Typical spectra from a map.  
 ~0.7s per spectrum

$d^2I/dV^2$  features lost in noise



Typical spectra for resolving  
 $d^2I/dV^2$  features  
 ~2s per spectrum

# GapMap

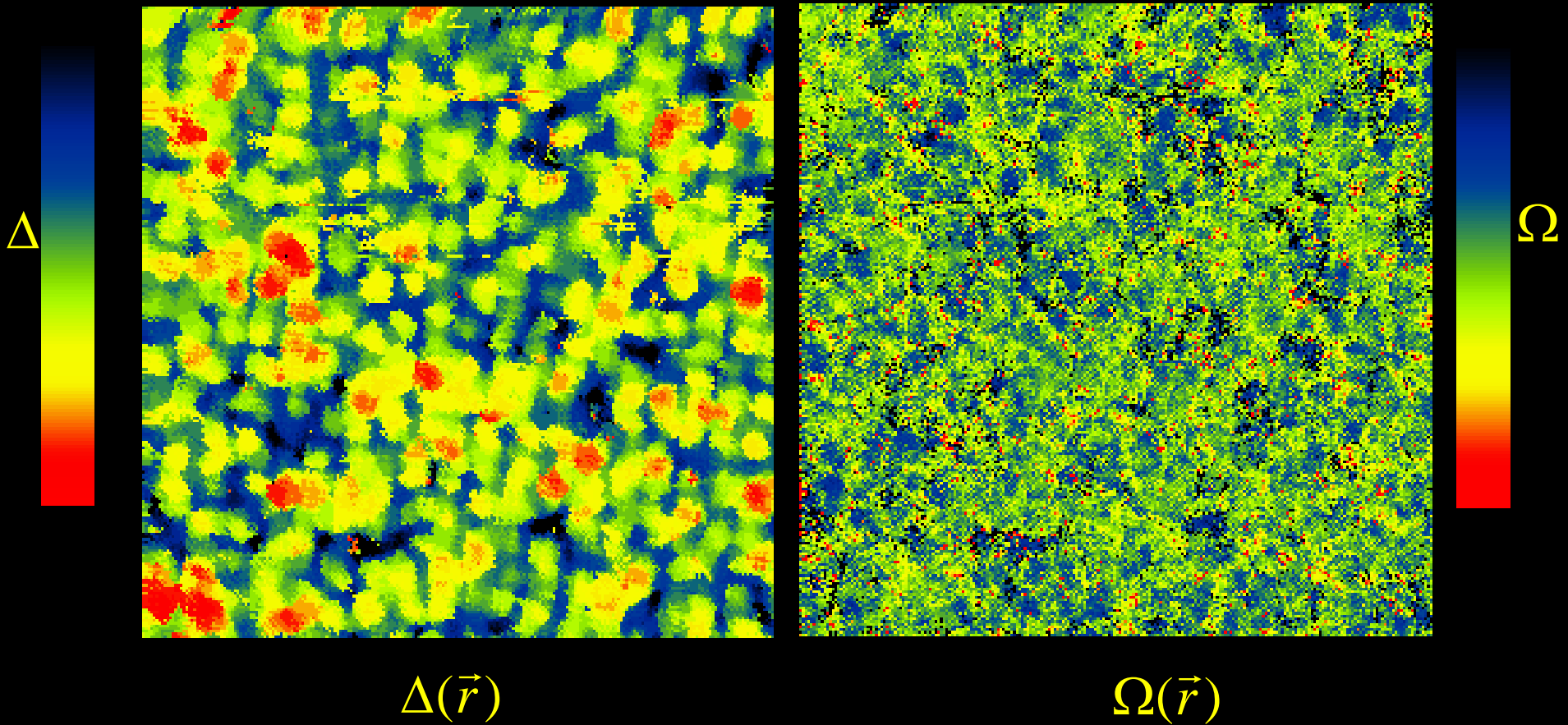


- Gapmap is inhomogeneous
- Features in  $d^2I/dV^2$  should be registered to the local value of  $\Delta(r)$



Subtracting the local  $\Delta(r)$  from peak in  $d^2I/dV^2$  is needed.

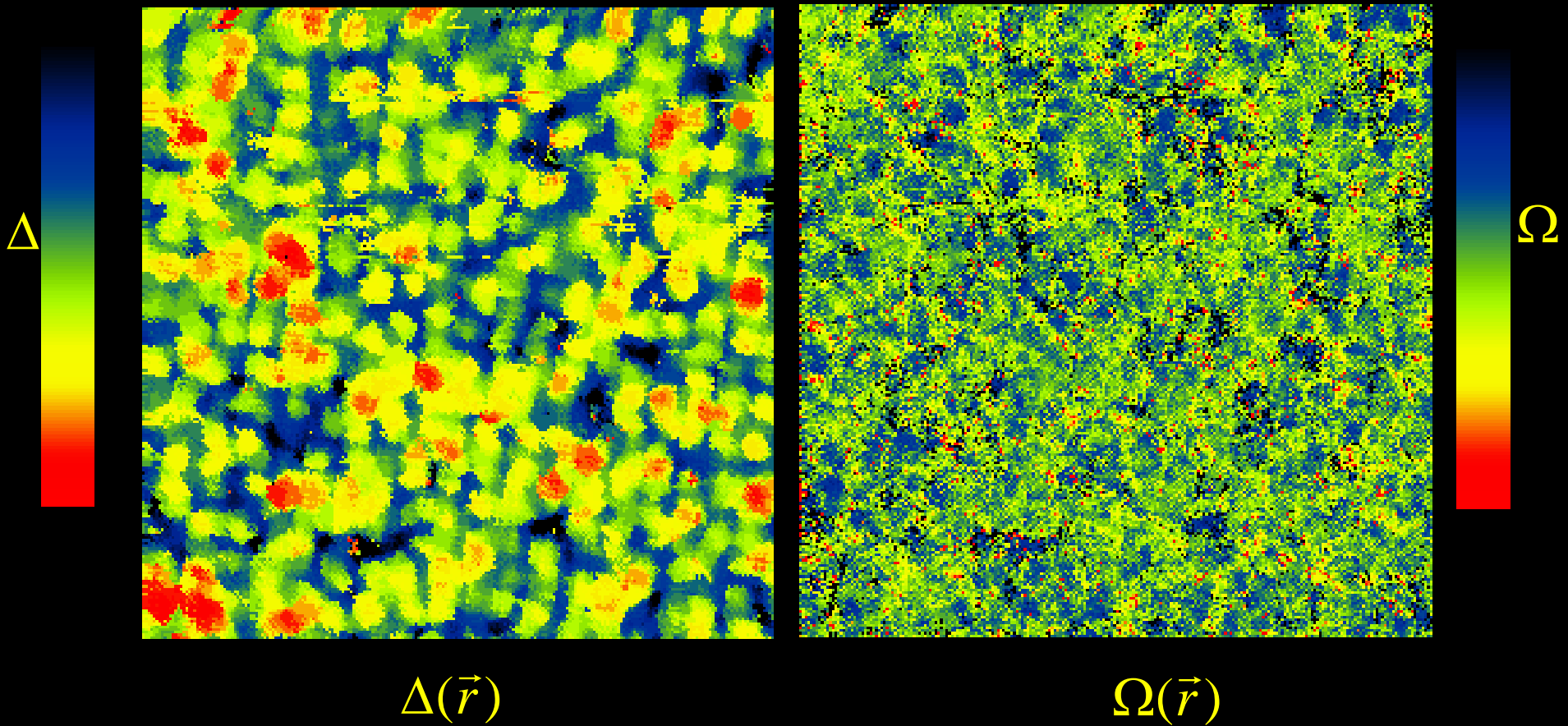
# GapMap – Omega Map



Results in an  $\Omega$  map where  

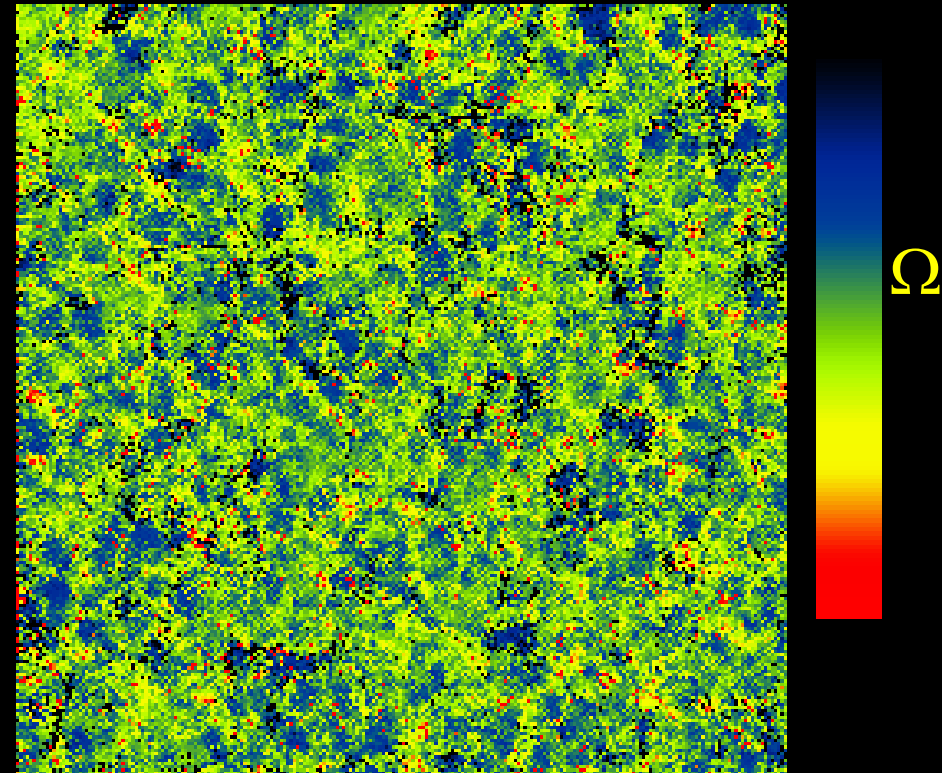
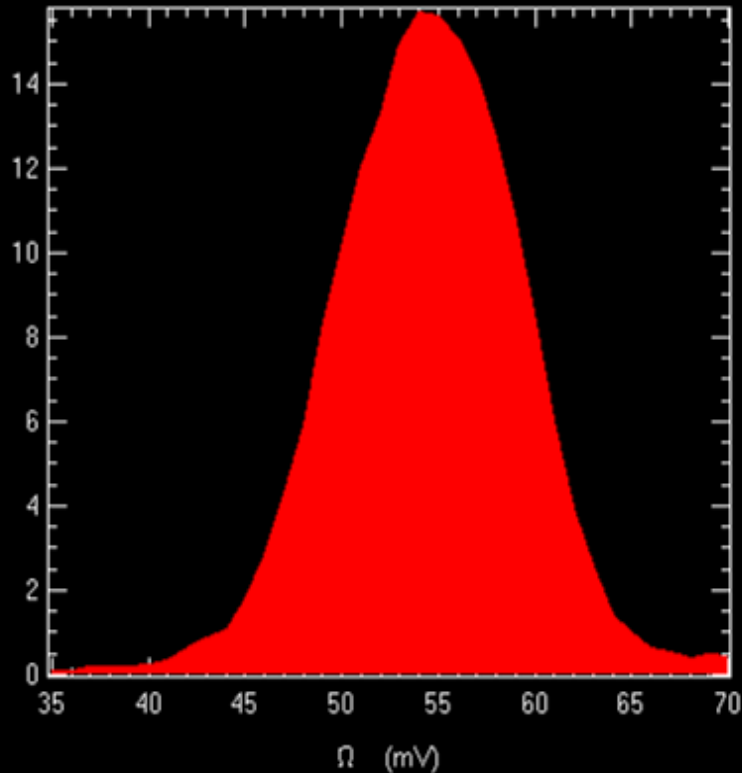
$$\Omega = E - \Delta$$

## GapMap – Omega Map



**$\Omega$  is inhomogeneous and weakly correlated  
with the gapmap**

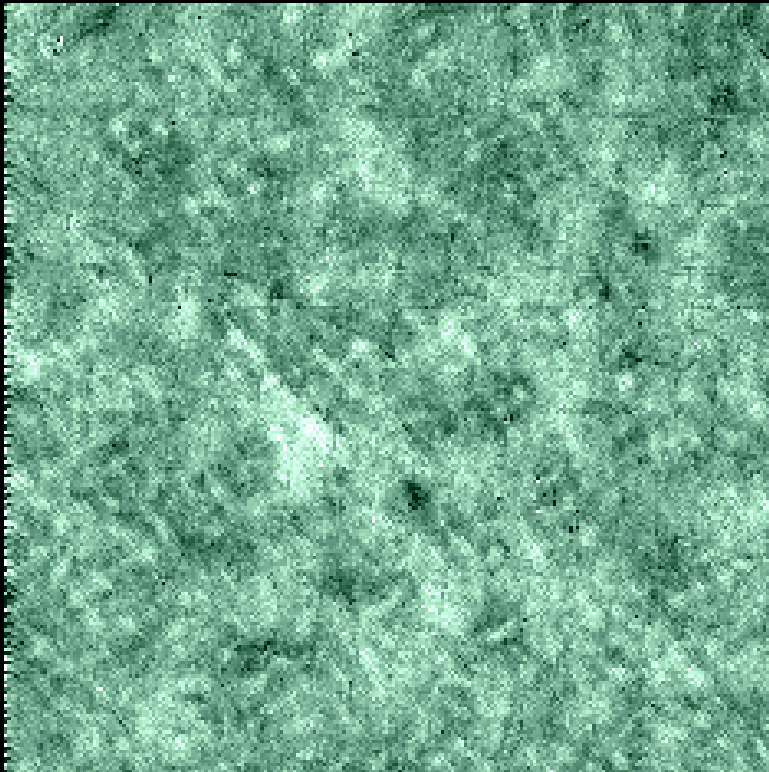
## GapMap – Omega Map



$$\Omega(\vec{r})$$

$\Omega$ 's distribution is peaked near 55 meV and  
 about 15 meV wide

$$g'(\vec{r}, \Omega) \equiv \frac{d^2 I}{dV^2}(\vec{r}, \Omega = eV - \Delta)$$

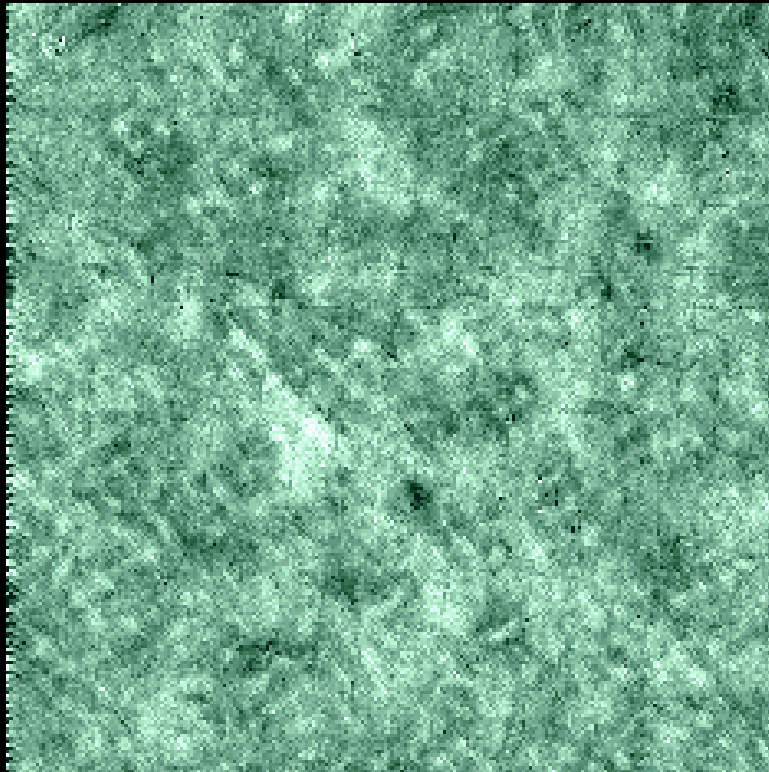


$$g'(\vec{r}, \Omega = -56 \text{ meV})$$

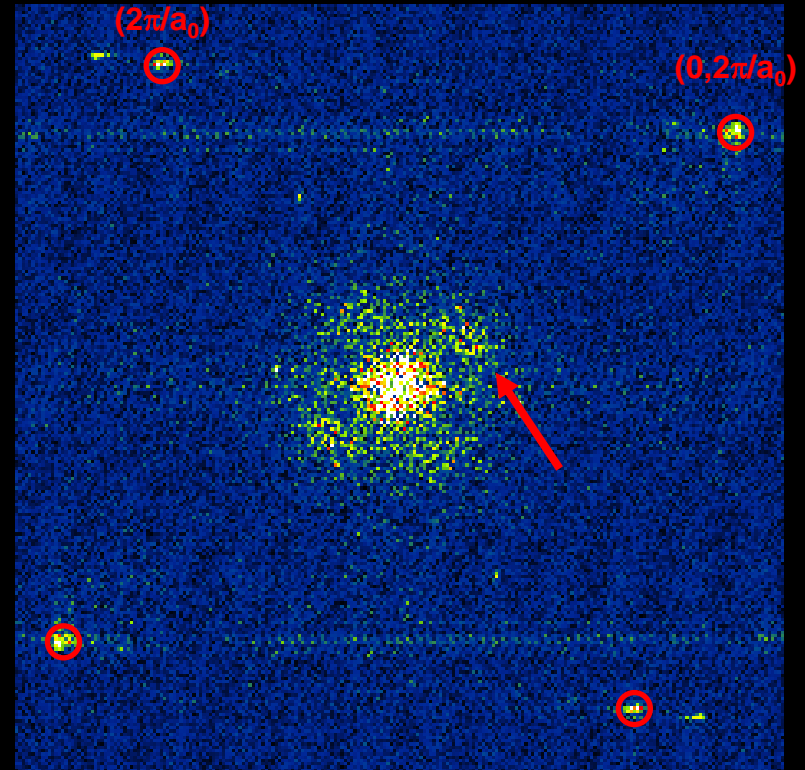
This is an image of the value of  $d^2 I / dV^2$  but now as a function of the energy of the boson  $\Omega = eV - \Delta$  after the disorder in  $\Delta(\vec{r})$  has been removed.

# FT-IETS *a la* Balatsky

$$g'(\vec{r}, \Omega) \xrightarrow{\text{FT}} g'(\vec{q}, \Omega)$$



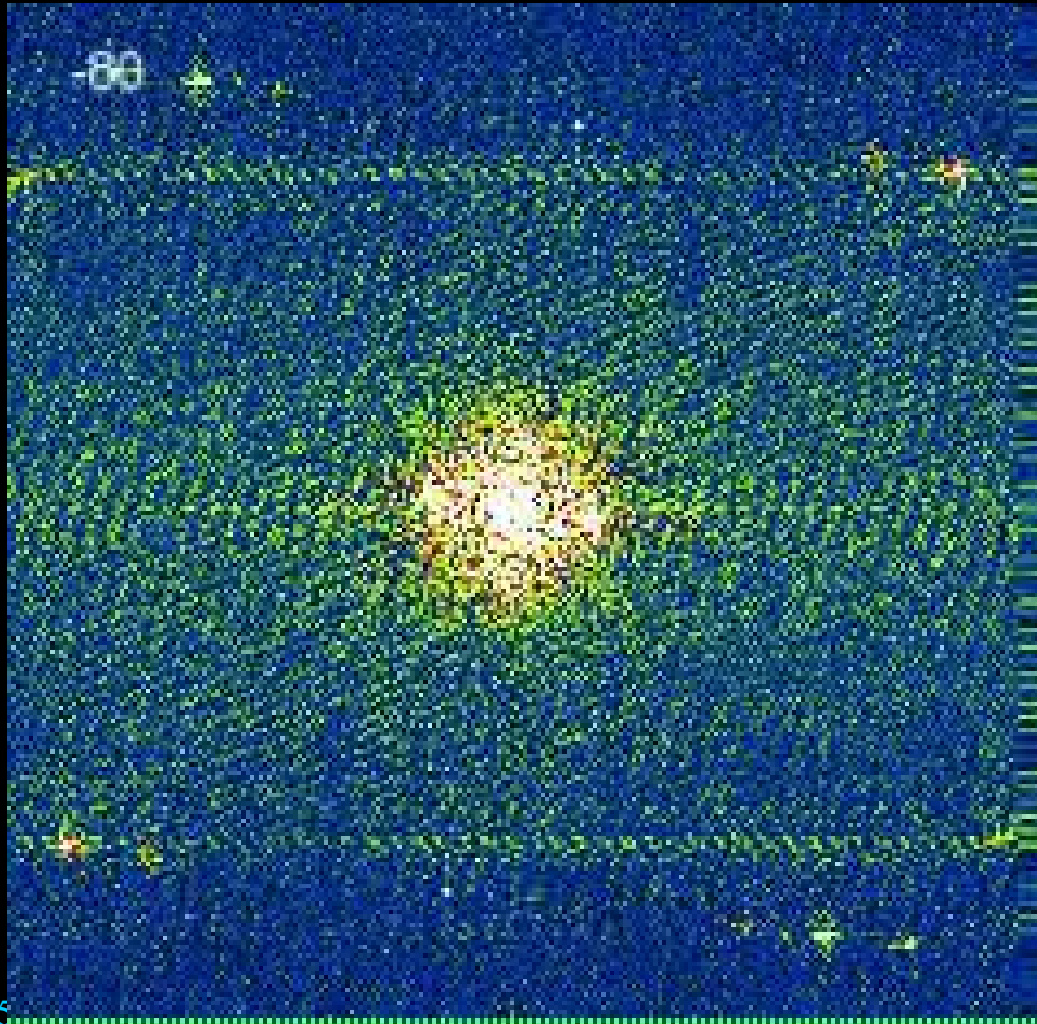
$g'(\vec{r}, \Omega = -56 \text{ meV})$

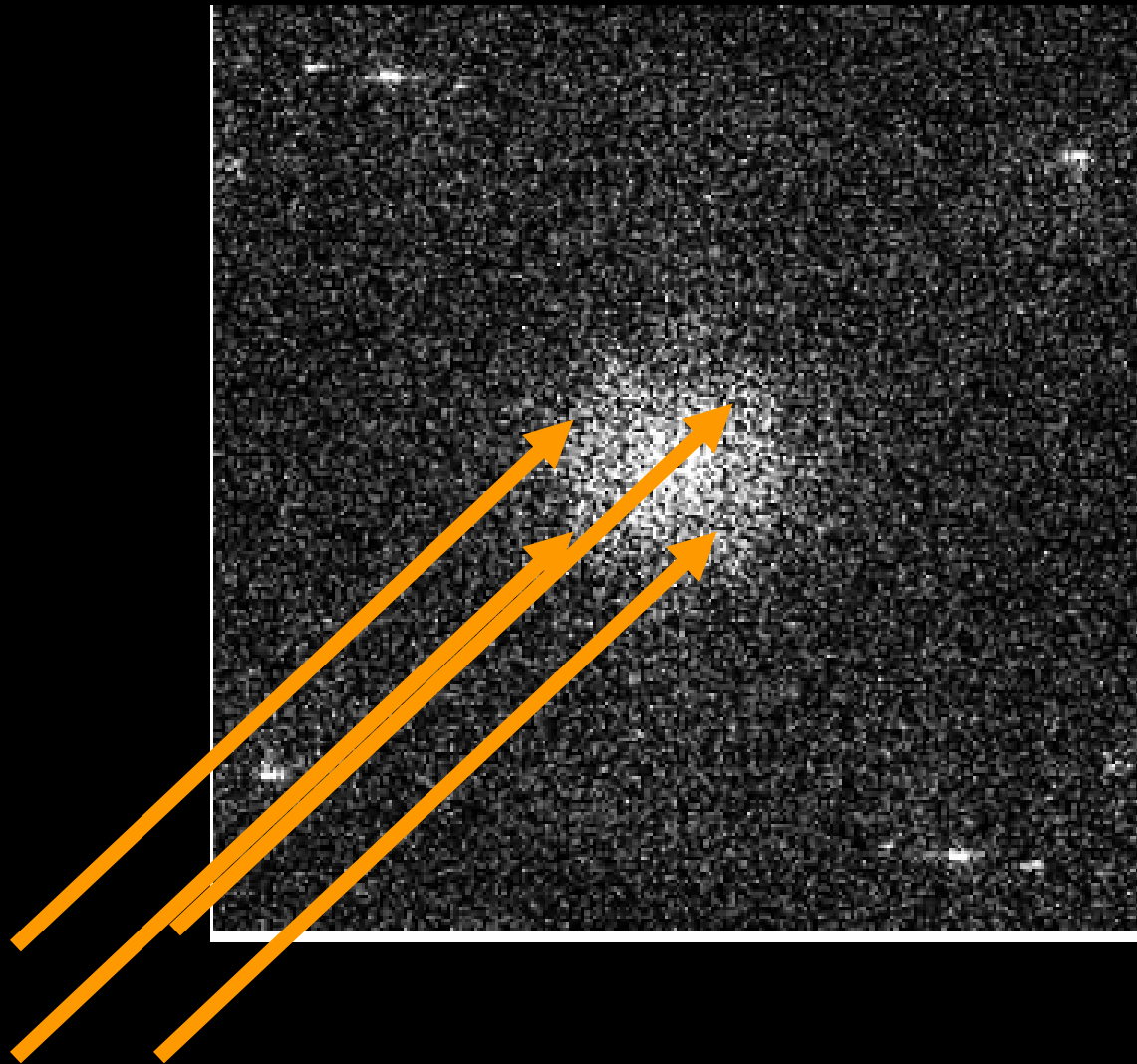


$g'(\vec{q}, \Omega = -56 \text{ meV})$

A peak in the FT-IETS is found corresponding to  $\lambda \sim 5a_0$  along  $\langle 1, 0 \rangle$

# *FT IETS energy dependence in BZ*





$\Omega(p)$  modulation, same  $v_1$  vectors are seen

## *Conclusion*

- We propose a new technique: Fourier Transform Inelastic Electron Tunneling Spectroscopy( FT IETS).
- Crucial part: careful measurement of  $d^2I/dV^2(p, eV)$
- Robust nature of IETS makes it a promising new spectroscopy tool. See Cornell STM data. Bosonic excitations are seen.
- Allows detection of both momentum and energy resolved Bosonic spectral function.
- Possible SC glue in cuprates. Remains to be seen. Definitely scatters electrons.